Supporting Information for:

Rapid Hydrogen Shift Scrambling in Hydroperoxy Substituted Organic Peroxy Radicals

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OH oxidation of CH_2=$CHCH_2CR_1HCH_3$

We have investigated the reaction between the CH_2=$CHCH_2CR_1HCH_3$ and the hydroxyl radical (OH) at the BHandHLYP/6-31+G(d,p) level of theory. The substituent R_1 is: an alcoholic (OH), a hydroperoxy (OOH) or a methoxy (OCH_3) group. The rate constants have been estimated with transition state theory including Eckart quantum tunneling correction. The OH radical can add to the outer (C1) and the inner (C2) carbon atom of the H_2C=C< or it can abstract a hydrogen atom from any of the other carbon atoms (C3, C4 or C5) or from the substituent R_1. (See Figure S1) The barrier heights for the OH addition reaction are lower than the ones for the H-abstraction reaction; furthermore, the barrier height for OH addition at the outer carbon atom in the H_2C=C< is lower than the one for OH addition at the inner carbon atom. We have computed the branching for each of the possible reaction pathways and they are tabulated in Table S1. The branching ratio for the reaction pathway is above 40 % for OH addition at the outer carbon atom in H_2**C**=C<, and we have only investigated the peroxy radicals $CH_2OHCH(OO)CH_2CR_1HCH_3$ formed after OH addition to the outer carbon atom and subsequent O_2 addition to inner carbon atom in the H_2C=**C**<. We expect a similar trend for the OH oxidation of CH_2=$CHCR_1HCH_2CH_3$ and CH_2=$CHCH_2CH_2CR_1H_2$ and have focused on the peroxy radicals formed after OH addition to the outer carbon atom followed by O2 additions to the inner carbon atom.

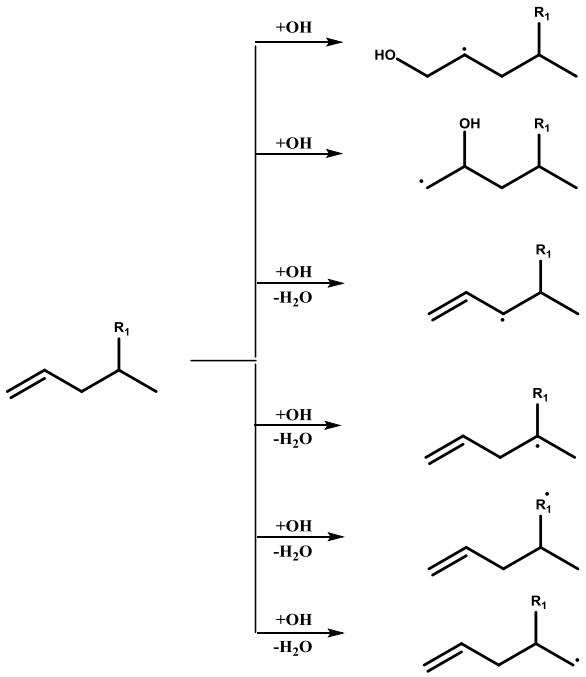


Figure S1. Schematic reaction mechanism of OH oxidation of CH_2=$CHCH_2CR_1HCH_3$.

Table S1: Branching ratio for the OH oxidation of CH_2=$CHCH_2CR_1HCH_3$

R_1	OH addition to C1	OH addition to C2	H-abstr. C3	H-abstr. C4	H-abstr. C5	H-abstr. R_1
H	49.83 %	39.07 %	8.36 %	2.20 %	0.55 %	-
OH	48.82 %	41.67 %	3.53 %	5.45 %	0.06 %	0.48 %
OOH	41.64 %	36.75 %	2.18 %	12.32 %	0.10 %	7.02 %
OCH_3	60.19 %	32.18 %	2.93 %	2.17 %	0.08 %	2.46 %

Rate constants for the H-shift reaction in the ROO_xOOH <-> ROOH_xOO cycle

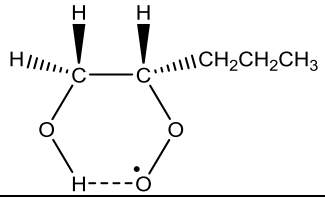
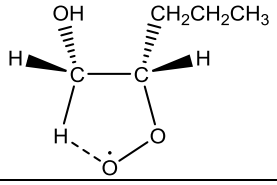
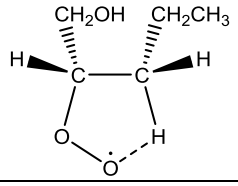
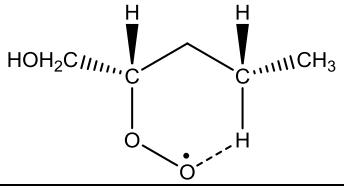
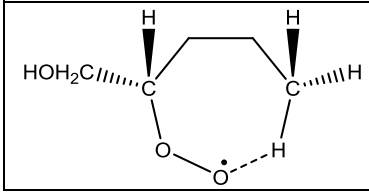
The M06-2X/aug-cc-pVTZ calculated parameters for H-shift reactions in the peroxy radical $HOCH_2CH(OO)CH_2CH_2CH_3$ in Table S2.

The M06-2X/aug-cc-pVTZ calculated parameters for H-shift reactions of the hydrogen atom attached to the oxygen atom in at the >CH(OO**H**) group in the peroxy radical ROO_xOOH in Table S3.
The M06-2X/aug-cc-pVTZ calculated parameters for selected H-shift reactions from the substituted peroxy radicals in Table S4

The CCSD(T)-F12a/VDZ-F12a//M06-2X/aug-cc-pVTZ calculated parameters for H-shift reactions in the ROO_xOOH <-> ROOH_xOO cycle are given in Table S5, S6 and S7 for ROO_3OOH, ROO_4OOH and ROO_5OOH, respectively.

The M06-2X/aug-cc-pVTZ calculated parameters for H-shift reactions in the ROO_xOOH <-> ROOH_xOO cycle are given in Table S8, S9 and S10 for ROO_3OOH, ROO_4OOH and ROO_5OOH, respectively.

Table S2. M06-2X/aug-cc-pVTZ calculated parameters for H-shift reactions in the peroxy radical $HOCH_2CH(OO)CH_2CH_2CH_3$

Structure of TS	H-shift	E_F[a]	E_R[b]	v_{imag}[c]	κ[d]	k_F[e]	k_R[f]
	1,5OH	21.1	1.0	1201i	6.5	4.5×10^{-3}	3.1×10^{12}
	1,4	32.1	23.8	2185i	2.3×10^{4}	2.2×10^{-7}	5.2×10^{-2}
	1,4	34.3	19.5	2119i	4.3×10^{3}	5.0×10^{-10}	17
	1,5	22.9	10.7	1782i	60	9.1×10^{-4}	5.6×10^{5}
	1,6	23.7	9.1	1909i	70	2.0×10^{-4}	2.0×10^{7}

[a] Forward barrier (ROO→ QOOH) in kcal mol^{-1}

[b] Reverse barrier (QOOH→ ROO) in kcal mol^{-1}

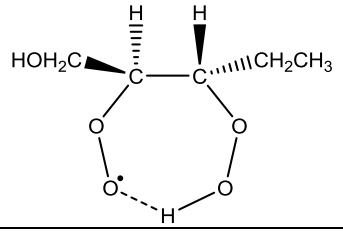
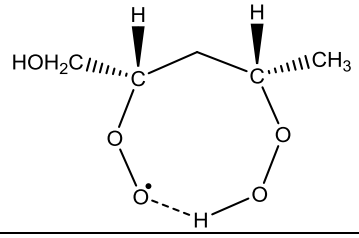
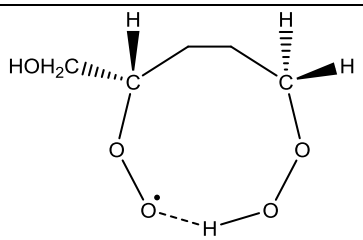
[c] Imaginary frequency in cm^{-1}

[d] Eckart quantum tunneling (unitless)

[e] Rate constant for the forward reaction (ROO→QOOH) in s^{-1}

[f] Rate constant for the reverse reaction (QOOH→ROO) in s^{-1}

Table S3. M06-2X/aug-cc-pVTZ calculated parameters for H-shift reactions of the hydrogen atom attached to the oxygen atom in at the >CH(OO**H**) group in the peroxy radical ROO_xOOH.

Structure of TS	xR_1	H-shift	E_F [a]	E_R [b]	ν_{imag} [c]	κ [d]	k_F [e]	k_R [f]
	3OOH	1,6	17.7	19.6	2683i	4.3×10^{4}	7.9×10^{3}	5.0×10^{2}
	4OOH	1,7	13.2	11.3	2191i	3.2×10^{2}	2.0×10^{5}	1.8×10^{6}
	5OOH	1,8	13.9	15.3	2337i	1.4×10^{3}	9.8×10^{4}	1.4×10^{4}

[a] Forward barrier (ROO→ QOOH) in kcal mol^{-1}

[b] Reverse barrier (QOOH→ ROO) in kcal mol^{-1}

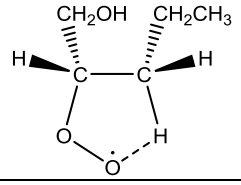
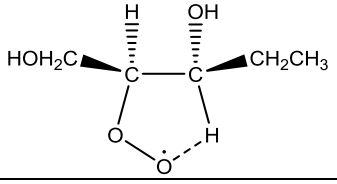
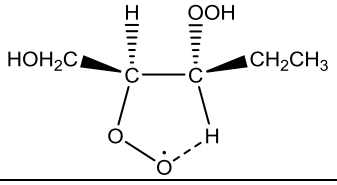
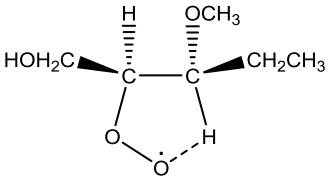
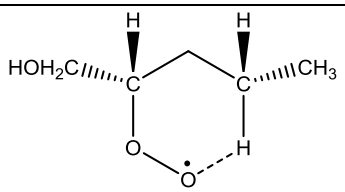
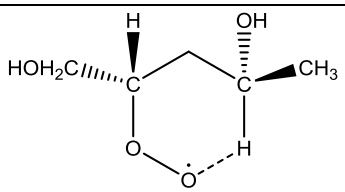
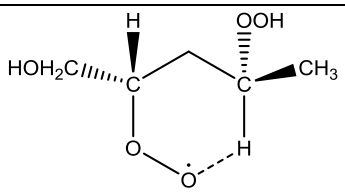
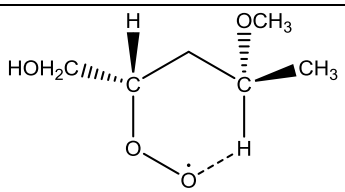
[c] Imaginary frequency in cm^{-1}

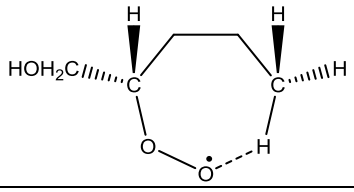
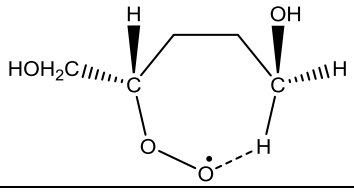
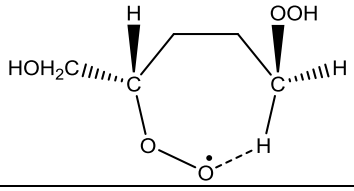
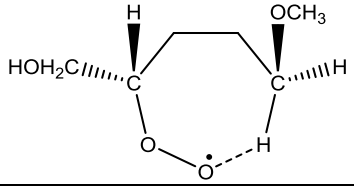
[d] Eckart quantum tunneling (unitless)

[e] Rate constant for the forward reaction (ROO→QOOH) in s^{-1}

[f] Rate constant for the reverse reaction (QOOH→ROO) in s^{-1}

Table S4. M06-2X/aug-cc-pVTZ calculated parameters for selected H-shift reactions from the substituted peroxy radicals.

Structure of TS	xR_1	H-shift	E_F[a]	E_R[b]	ν_{imag}[c]	κ[d]	k_F[e]	k_R[f]
	3H	1,4	34.3	19.5	2119i	4.3×10^{3}	5.0×10^{-10}	17
	3OH	1,4	27.3	19.6	1789i	2.7×10^{2}	7.0×10^{-6}	8.4×10^{-1}
	3OOH	1,4	30.1	60.2	1829i	3.2×10^{3}	6.2×10^{-7}	-
	$3OCH_3$	1,4	25.2	18.3	1805i	2.4×10^{2}	1.2×10^{-4}	7.6
	4H	1,5	22.9	10.7	1782i	60	6.9×10^{-4}	5.6×10^{5}
	4OH	1,5	16.8	11.3	1531i	20	16	6.5×10^{4}
	4OOH	1,5	23.1	50.4	1454i	32	1.1×10^{-3}	-
	$4OCH_3$	1,5	18.6	15.2	1642i	50	3.9×10^{-1}	4.2×10^{2}

	5H	1,6	23.7	9.1	1909i	70	$2.0x10^{-4}$	$2.0x10^{7}$
	5OH	1,6	18.6	11.0	1840i	80	5.3	$9.9x10^{5}$
	5OOH	1,6	20.2	48.2	1895i	$9.2x10^{2}$	4.0	-
	$5OCH_3$	1,6	17.7	10.9	1873i	90	4.4	$3.1x10^{6}$

[a] Forward barrier (ROO→ QOOH) in kcal mol^{-1}

[b] Reverse barrier (QOOH→ ROO) in kcal mol^{-1}

[c] Imaginary frequency in cm^{-1}

[d] Eckart quantum tunneling (unitless)

[e] Rate constant for the forward reaction (ROO→QOOH) in s^{-1}

[f] Rate constant for the reverse reaction (QOOH→ROO) in s^{-1}

Table S5. CCSD(T)-F12a/VDZ-F12a//M06-2X/aug-cc-pVTZ calculated parameters for H-shift reactions in the ROO_3OOH <-> ROOH_3OO cycle

H-shift	E_F[a]	E_R[b]	ν_{imag}[c]	κ[d]	k_f[e]	k_r[f]
1,4 in ROO_3OOH	28.4	60.1	1829i	2.4×10^{3}	8.2×10^{-6}	-
1,5 in ROO_3OOH	23.8	8.9	1822i	48	1.8×10^{-4}	6.7×10^{6}
1,6 in ROO_3OOH	23.9	7.7	1910i	47	7.4×10^{-5}	3.4×10^{7}
ROO_3OOH <-> ROOH_3OO	16.5	18.0	2683i	2.3×10^{4}	2.9×10^{4}	3.8×10^{3}
1,4 in ROOH_3OO	30.1	59.0	2061i	6.1×10^{4}	4.2×10^{-5}	-
1,5 in ROOH_3OO	20.6	10.9	1733i	49	5.5×10^{-2}	3.1×10^{5}

[a] Forward barrier (ROO→ QOOH) in kcal mol^{-1}
[b] Reverse barrier (QOOH→ ROO) in kcal mol^{-1}
[c] Imaginary frequency in cm^{-1}
[d] Eckart quantum tunneling (unitless)
[e] Rate constant for the forward reaction (ROO→QOOH) in s^{-1}
[f] Rate constant for the reverse reaction (QOOH→ROO) in s^{-1}

Table S6. CCSD(T)-F12a/VDZ-F12a//M06-2X/aug-cc-pVTZ calculated parameters for H-shift reactions in the ROO_4OOH <-> ROOH_4OO cycle.

H-shift	E_F[a]	E_R[b]	ν_{imag}[c]	κ[d]	k_f[e]	k_r[f]
1,4 in ROO_4OOH	34.7	20.9	2149i	8.3×10^{3}	1.9×10^{-9}	22
1,5 in ROO_4OOH	21.5	51.1	1454i	30	1.5×10^{-2}	-
1,6 in ROO_4OOH	28.9	11.0	1855i	89	6.7×10^{-7}	8.1×10^{6}
ROO_4OOH <-> ROOH_4OO	12.6	10.8	2191i	2.7×10^{2}	4.7×10^{5}	3.4×10^{6}
1,5 in ROOH_4OO	20.4	51.6	1877i	8.3×10^{2}	7.9	-
1,6 in ROO_4OO	20.9	12.0	1724i	56	1.4×10^{-2}	4.9×10^{4}

[a] Forward barrier (ROO→ QOOH) in kcal mol^{-1}
[b] Reverse barrier (QOOH→ ROO) in kcal mol^{-1}
[c] Imaginary frequency in cm^{-1}
[d] Eckart quantum tunneling (unitless)
[e] Rate constant for the forward reaction (ROO→QOOH) in s^{-1}
[f] Rate constant for the reverse reaction (QOOH→ROO) in s^{-1}

Table S7. CCSD(T)-F12a/VDZ-F12a//M06-2X/aug-cc-pVTZ calculated parameters for H-shift reactions in the ROO_5OOH <-> ROOH_5OO cycle.

H-shift	E_F[a]	E_R[b]	ν_{imag}[c]	κ[d]	k_f[e]	k_r[f]
1,4 in ROO_5OOH	31.0	19.9	2042i	2.4×10^{3}	5.9×10^{-8}	3.6
1,5 in ROO_5OOH	22.0	8.6	1811i	43	9.0×10^{-3}	6.6×10^{7}
1,6 in ROO_5OOH	19.7	49.8	1895i	8.3×10^{2}	8.0	-
ROO_5OOH <-> ROOH_5OO	14.3	15.7	2337i	1.6×10^{3}	5.6×10^{4}	8.8×10^{3}
1,5 in ROOH_5OO	24.5	9.3	1858i	60	1.8×10^{-4}	9.0×10^{6}
1,6 in ROOH_5OO	21.6	54.2	1912i	1.5×10^{3}	1.2	-
1,7 in ROOH_5OO	22.1	12.5	1836i	1.1×10^{2}	2.4×10^{-3}	3.3×10^{4}

[a] Forward barrier (ROO→ QOOH) in kcal mol^{-1}

[b] Reverse barrier (QOOH→ ROO) in kcal mol^{-1}

[c] Imaginary frequency in cm^{-1}

[d] Eckart quantum tunneling (unitless)

[e] Rate constant for the forward reaction (ROO→QOOH) in s^{-1}

[f] Rate constant for the reverse reaction (QOOH→ROO) in s^{-1}

Table S8. M06-2X/aug-cc-pVTZ calculated parameters for H-shift reactions in the ROO_3OOH <-> ROOH_3OO cycle

H-shift	E_F[a]	E_R[b]	ν_{imag}[c]	κ[d]	k_f[e]	k_r[f]
1,4 in ROO_3OOH	30.1	60.2	1829i	3.2×10^{3}	6.2×10^{-7}	-
1,5 in ROO_3OOH	23.8	10.1	1822i	63	2.4×10^{-4}	1.1×10^{6}
1,6 in ROO_3OOH	23.6	8.1	1910i	53	1.5×10^{-4}	2.0×10^{7}
ROO_3OOH <-> ROOH_3OO	17.7	19.6	2683i	4.3×10^{4}	7.9×10^{3}	5.0×10^{2}
1,4 in ROOH_3OO	32.3	59.2	2061i	1.0×10^{5}	1.5×10^{-6}	-
1,5 in ROOH_3OO	21.6	12.3	1733i	62	1.3×10^{-2}	3.8×10^{4}

[a] Forward barrier (ROO→ QOOH) in kcal mol^{-1}
[b] Reverse barrier (QOOH→ ROO) in kcal mol^{-1}
[c] Imaginary frequency in cm^{-1}
[d] Eckart quantum tunneling (unitless)
[e] Rate constant for the forward reaction (ROO→QOOH) in s^{-1}
[f] Rate constant for the reverse reaction (QOOH→ROO) in s^{-1}

Table S9. M06-2X/aug-cc-pVTZ calculated parameters for H-shift reactions in the ROO_4OOH <-> ROOH_4OO cycle.

H-shift	E_F[a]	E_R[b]	ν_{imag}[c]	κ[d]	k_f[e]	k_r[f]
1,4 in ROO_4OOH	36.7	23.5	2149i	1.8×10^{4}	1.3×10^{-10}	5.9×10^{-1}
1,5 in ROO_4OOH	23.1	50.4	1454i	32	1.1×10^{-3}	-
1,6 in ROO_4OOH	29.8	12.4	1855i	1.2×10^{2}	1.9×10^{-7}	1.1×10^{6}
ROO_4OOH <-> ROOH_4OO	13.2	11.3	2191i	3.2×10^{2}	2.0×10^{5}	1.8×10^{6}
1,5 in ROOH_4OO	22.0	51.2	1877i	1.2×10^{3}	7.0×10^{-1}	-
1,6 in ROO_4OO	21.4	12.1	1724i	57	6.8×10^{-3}	4.0×10^{4}

[a] Forward barrier (ROO→ QOOH) in kcal mol^{-1}
[b] Reverse barrier (QOOH→ ROO) in kcal mol^{-1}
[c] Imaginary frequency in cm^{-1}
[d] Eckart quantum tunneling (unitless)
[e] Rate constant for the forward reaction (ROO→QOOH) in s^{-1}
[f] Rate constant for the reverse reaction (QOOH→ROO) in s^{-1}

Table S10. M06-2X/aug-cc-pVTZ calculated parameters for H-shift reactions in the ROO_5OOH <-> ROOH_5OO cycle.

H-shift	E_F[a]	E_R[b]	ν_{imag}[c]	κ[d]	k_f[e]	k_r[f]
1,4 in ROO_5OOH	33.1	22.6	2042i	4.8×10^{3}	3.3×10^{-9}	6.7×10^{-2}
1,5 in ROO_5OOH	22.8	10.6	1811i	67	3.6×10^{-3}	3.6×10^{6}
1,6 in ROO_5OOH	20.2	48.2	1895i	9.2×10^{2}	4.0	-
ROO_5OOH <-> ROOH_5OO	13.9	15.3	2337i	1.4×10^{3}	9.8×10^{4}	1.4×10^{4}
1,5 in ROOH_5OO	25.7	11.3	1858i	97	3.8×10^{-5}	4.9×10^{5}
1,6 in ROOH_5OO	22.4	53.5	1912i	1.8×10^{3}	3.4×10^{-1}	-
1,7 in ROOH_5OO	21.4	11.7	1836i	61	4.9×10^{-3}	7.0×10^{4}

[a] Forward barrier (ROO→ QOOH) in kcal mol^{-1}

[b] Reverse barrier (QOOH→ ROO) in kcal mol^{-1}

[c] Imaginary frequency in cm^{-1}

[d] Eckart quantum tunneling (unitless)

[e] Rate constant for the forward reaction (ROO→QOOH) in s^{-1}

[f] Rate constant for the reverse reaction (QOOH→ROO) in s^{-1}

Atmospheric impact of ROO_5OOH

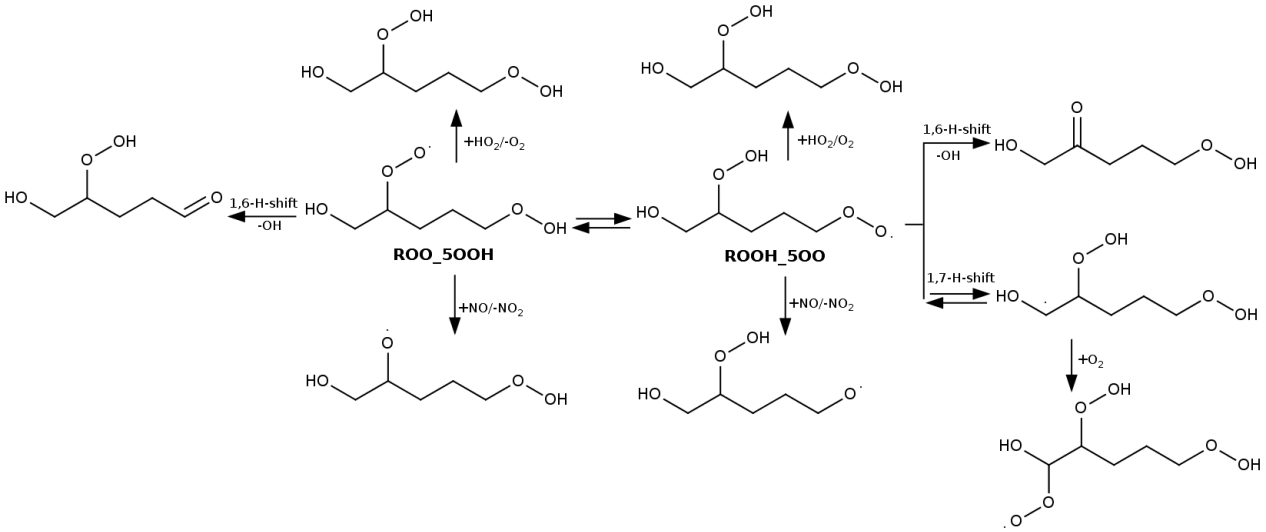


Figure S2. The reaction scheme for the atmospheric degradation of the peroxy radical ROO_5OOH. Only dominant H-shift reactions are shown.

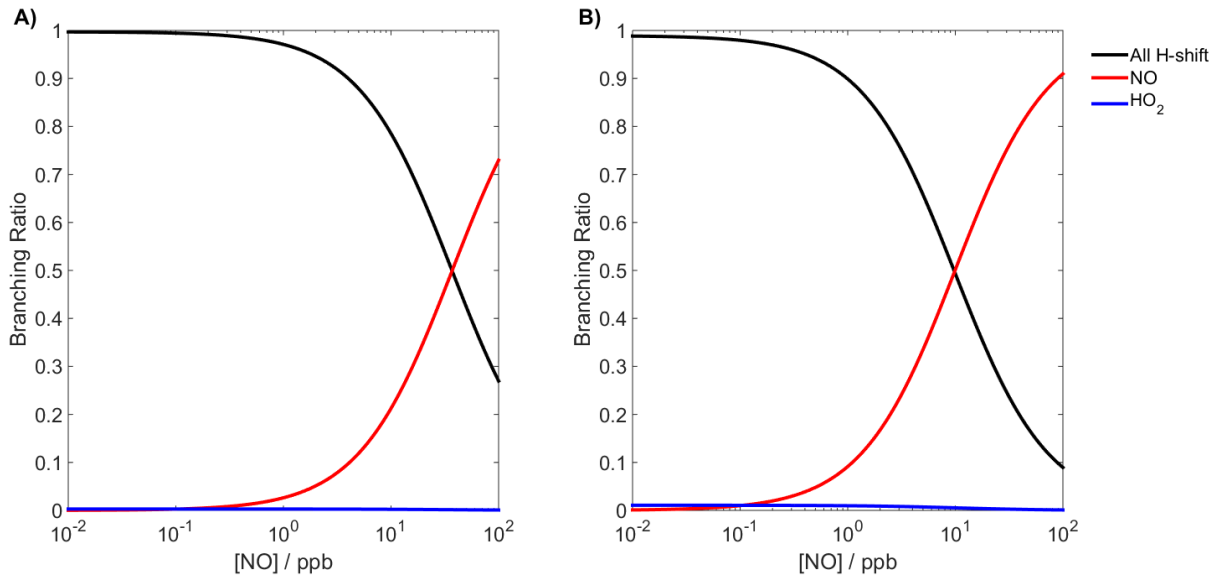


Figure S3. The atmospheric degradation of the peroxy radical ROO_5OOH. The branching ratios of the products formed from either reaction with NO (red) or HO_2 (blue) or the sum of all the H-shift reactions (black) as a function of the concentration of NO. The concentration of HO_2 is held constant at 55 ppt. Panel A) shows the branching ratios without the H-shift reaction ROO_5OOH <-> ROOH_5OO and panel B) shows how the branching ratios change with inclusion of this H-shift reaction.

The expectation value of the total spin $<S^2>$ and T_1 diagonostic values:

The expectation value of the total spin deviated less than 2% from the expected value of $<S^2>$ = ¾ before spin annihilation, and the expectation value is close to 0.7500 after spin annihilation.

Table S11. $<S^2>$ values in the H-shift reactions in the peroxy radical $HOCH_2CH(OO)CR_1HCH_2CH_3$.

Species	$<S^2>$ before spin annihilation	$<S^2>$ after spin annihilation
Reactant	0.7558	0.7500
1,5 OH TS	0.7596	0.7501
1,5 OH P	0.7560	0.7500
1,4 Outer TS	0.7622	0.7501
1,4 Outer P	0.7551	0.7500
1,4 TS	0.7616	0.7501
1,4 P	0.7552	0.7500
1,5 TS	0.7592	0.7500
1,5 P	0.7553	0.7500
1,6 TS	0.7601	0.7501
1,6 P	0.7553	0.7500

Table S12. $<S^2>$ values in the H-shift reactions in the peroxy radicals, $HOCH_2CH(OO)CR_1HCH_2CH_3$, $HOCH_2CH(OO)CH_2CR_1HCH_3$ and $HOCH_2CH(OO)CH_2CH_2CR_1H_2$, where R_1=OH.

Species	$<S^2>$ before spin annihilation	$<S^2>$ after spin annihilation
1,4 in ROO_3OH R	0.7558	0.7500
1,4 in ROO_3OH TS	0.7607	0.7501
1,4 in ROO_3OH P	0.7542	0.7500
1,5 in ROO_4OH R	0.7558	0.7500
1,5 in ROO_4OH TS	0.7591	0.7500
1,5 in ROO_4OH P	0.7546	0.7500
1,6 in ROO_5OH R	0.7557	0.7500
1,6 in ROO_5OH TS	0.7596	0.7500
1,6 in ROO_5OH P	0.7547	0.7500

Table S13. $<S^2>$ values in the H-shift reactions in the peroxy radicals, $HOCH_2CH(OO)CR_1HCH_2CH_3$, $HOCH_2CH(OO)CH_2CR_1HCH_3$ and $HOCH_2CH(OO)CH_2CH_2CR_1H_2$, where R_1=OCH_3.

Species	$<S^2>$ before spin annihilation	$<S^2>$ after spin annihilation
1,4 in ROO_3OCH_3 R	0.7557	0.7500
1,4 in ROO_3OCH_3 TS	0.7607	0.7501
1,4 in ROO_3OCH_3 P	0.7545	0.7500
1,5 in ROO_4OCH_3 R	0.7558	0.7500
1,5 in ROO_4OCH_3 TS	0.7591	0.7500
1,5 in ROO_4OCH_3 P	0.7545	0.7500
1,6 in ROO_5OCH_3 R	0.7558	0.7500
1,6 in ROO_5OCH_3 TS	0.7597	0.7500
1,6 in ROO_5OCH_3 P	0.7545	0.7500

Table S14. $<S^2>$ values in the ROO_3OOH <-> ROOH_3OO cycle.

Species	$<S^2>$ before spin annihilation	$<S^2>$ after spin annihilation
Reactant in ROO_3OOH	0.7557	0.7500
1,4 in ROO_3OOH TS	0.7611	0.7501
1,5 in ROO_3OOH TS	0.7596	0.7500
1,5 in ROO_3OOH P	0.7554	0.7500
1,6 in ROO_3OOH TS	0.7599	0.7500
1,6 in ROO_3OOH P	0.7552	0.7500
1,6 OOH in ROO_3OOH TS	0.7617	0.7501
1,6 OOH in ROO_3OOH P	0.7556	0.7500
1,4 in ROOH_3OO TS	0.7620	0.7501
1,5 in ROOH_3OO TS	0.7599	0.7500
1,5 in ROOH_3OO P	0.7545	0.7500

Table S15. $<S^2>$ values in the ROO_4OOH <-> ROOH_4OO cycle.

Species	$<S^2>$ before spin annihilation	$<S^2>$ after spin annihilation
Reactant in ROO_4OOH	0.7558	0.7500
1,4 in ROO_4OOH TS	0.7617	0.7501
1,4 in ROO_4OOH P	0.7559	0.7500
1,5 in ROO_4OOH TS	0.7593	0.7500
1,6 in ROO_4OOH TS	0.7609	0.7500
1,6 in ROO_4OOH P	0.7553	0.7500
1,7 OOH in ROO_4OOH TS	0.7609	0.7501
1,7 OOH in ROO_4OOH P	0.7558	0.7500
1,5 in ROOH_4OO TS	0.7598	0.7500
1,6 in ROOH_4OO TS	0.7600	0.7500
1,6 in ROOH_4OO P	0.7547	0.7500

Table S16. $<S^2>$ values in the ROO_5OOH <-> ROOH_5OO cycle.

Species	$<S^2>$ before spin annihilation	$<S^2>$ after spin annihilation
Reactant in ROO_5OOH	0.7558	0.7500
1,4 in ROO_5OOH TS	0.7614	0.7501
1,4 in ROO_5OOH P	0.7557	0.7500
1,5 in ROO_5OOH TS	0.7596	0.7500
1,5 in ROO_5OOH P	0.7557	0.7500
1,6 in ROO_5OOH TS	0.7598	0.7500
1,8 OOH in ROO_5OOH TS	0.7614	0.7501
1,8 OOH in ROO_5OOH P	0.7558	0.7500
1,5 in ROOH_5OO TS	0.7597	0.7501
1,5 in ROOH_5OO P	0.7557	0.7500
1,6 in ROOH_5OO TS	0.7600	0.7501
1,7 in ROOH_5OO TS	0.7594	0.7500
1,7 in ROOH_5OO P	0.7547	0.7500

Table S17. T1-diagnostics in the H-shift reactions in the peroxy radicals, $HOCH_2CH(OO)CR_1HCH_2CH_3$, $HOCH_2CH(OO)CH_2CR_1HCH_3$ and $HOCH_2CH(OO)CH_2CH_2CR_1H_2$, where R_1=H.

Species	T_1-diagnostic value
Reactant	0.02403718
1,4 outer TS	0.02563546
1,4 outer P	0.01364011
1,4 TS	0.02105024
1,4 P	0.01189529
1,5 TS	0.01879984
1,5 P	0.01211440
1,6 TS	0.01794728
1,6 P	0.01177724

Table S18. T1-diagnostics in the H-shift reactions in the peroxy radicals, $HOCH_2CH(OO)CR_1HCH_2CH_3$, $HOCH_2CH(OO)CH_2CR_1HCH_3$ and $HOCH_2CH(OO)CH_2CH_2CR_1H_2$, where R_1=OH.

Species	T_1-diagnostic value
1,4 in ROO_3OH R	0.02286110
1,4 in ROO_3OH TS	0.02555850
1,4 in ROO_3OH P	0.01374336
1,5 in ROO_4OH R	0.02298385
1,5 in ROO_4OH TS	0.01879984
1,5 in ROO_4OH P	0.01211440
1,6 in ROO_5OH R	0.02293042
1,6 in ROO_5OH TS	0.01662807
1,6 in ROO_5OH P	0.01304807

Table S19. T1-diagnostics in the H-shift reactions in the peroxy radicals, $HOCH_2CH(OO)CR_1HCH_2CH_3$, $HOCH_2CH(OO)CH_2CR_1HCH_3$ and $HOCH_2CH(OO)CH_2CH_2CR_1H_2$, where R_1=OCH_3.

Species	T_1-diagnostic value
1,4 in ROO_3OCH_3 R	0.02211266
1,4 in ROO_3OCH_3 TS	0.02547088
1,4 in ROO_3OCH_3 P	0.01383294
1,5 in ROO_4OCH_3 R	0.02246540
1,5 in ROO_4OCH_3 TS	0.01627742
1,5 in ROO_4OCH_3 P	0.01350623
1,6 in ROO_5OCH_3 R	0.02209254
1,6 in ROO_5OCH_3 TS	0.01664942
1,6 in ROO_5OCH_3 P	0.01344712

Table S20. T1-diagnostics for the ROO_3OOH <-> ROOH_3OO cycle

Species	T_1-diagnostic value
Reactant in ROO_3OOH	0.02157542
1,4 in ROO_3OOH TS	0.02750971
1,5 in ROO_3OOH TS	0.01766327
1,5 in ROO_3OOH P	0.01244534
1,6 in ROO_3OOH TS	0.01669240
1,6 in ROO_3OOH P	0.01193185
1,6 OOH in ROO_3OOH TS	0.03719980
1,6 OOH in ROO_3OOH P	0.02248532
1,4 in ROOH_3OO TS	0.02336986
1,5 in ROOH_3OO TS	0.01851522
1,5 in ROOH_3OO P	0.01377997

Table S21. T1-diagnostics for the ROO_4OOH <-> ROOH_4OO cycle

Species	T_1-diagnostic value
Reactant in ROO_4OOH	0.02235318
1,4 in ROO_4OOH TS	0.02046672
1,4 in ROO_4OOH P	0.01267873
1,5 in ROO_4OOH TS	0.02187458
1,5 in ROO_4OOH P	0.01268080
1,6 in ROO_4OOH TS	0.03059393
1,6 in ROO_4OOH P	0.01202866
1,7 OOH in ROO_4OOH TS	0.03059393
1,7 OOH in ROO_4OOH P	0.02295192
1,5 in ROOH_4OO TS	0.01679175
1,5 in ROOH_4OO P	0.01278347
1,6 in ROOH_4OO TS	0.01886424
1,6 in ROOH_4OO P	0.01369826

Table S22. T1-diagnostics for the ROO_5OOH <-> ROOH_5OO cycle

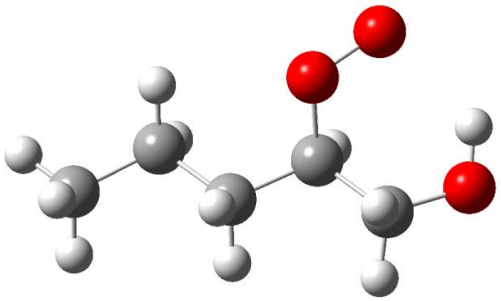
Species	T_1-diagnostic value
Reactant in ROO_5OOH	0.02213214
1,4 in ROO_5OOH TS	0.02055459
1,4 in ROO_5OOH P	0.01236938
1,5 in ROO_5OOH TS	0.01727393
1,5 in ROO_5OOH P	0.01280208
1,6 in ROO_5OOH TS	0.01638659
1,6 in ROO_5OOH P	0.01262329
1,8 OOH in ROO_5OOH TS	0.04226878
1,8 OOH in ROO_5OOH P	0.02227608
1,5 in ROOH_5OO TS	0,01893107
1,5 in ROOH_5OO P	0.01234746
1,6 in ROOH_5OO TS	0.01599103
1,6 in ROOH_5OO P	0.01294801
1,7 in ROOH_5OO TS	0.01656457
1,7 in ROOH_5OO P	0.01368813

Optimized Geometries:

The M06-2X/aug-cc-pVTZ optimized geometries (x, y, and z in Ångstrøm) for the conformer with the lowest zero-point corrected energy.

M06-2X/aug-cc-pVTZ calculated geometry coordinates for H-shift reactions peroxy radical HOCH2CH(OO)CHHCH2CH3.

HOCH2CH(OO)CHHCH2CH3



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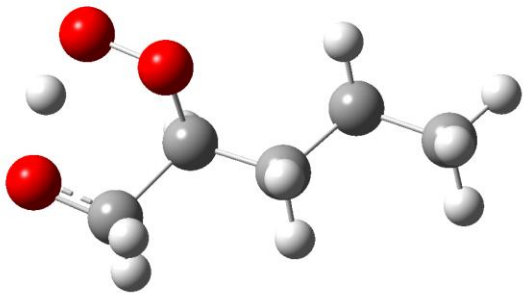
1,5 OH TS



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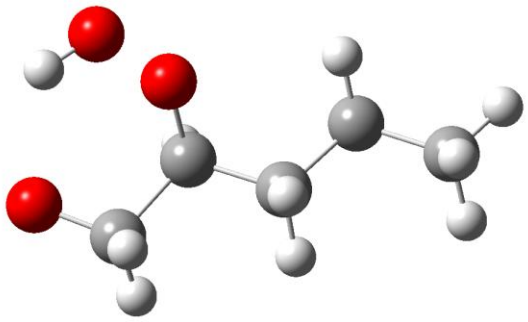
1,5 OH P



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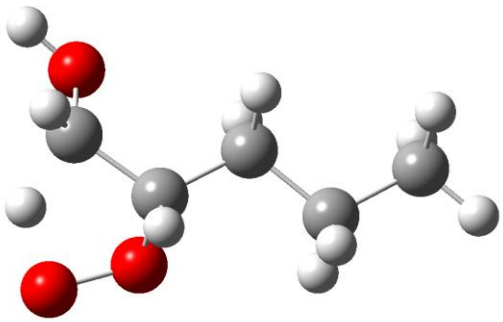
1,4 outer TS



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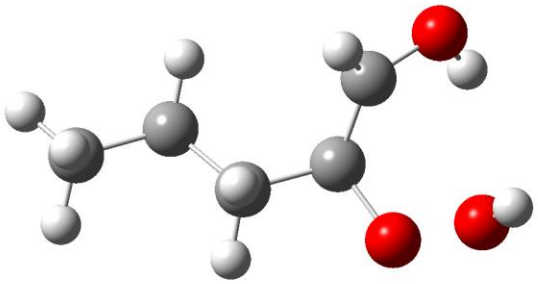
1,4 outer P



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H -1.105055 -0.529209 1.324179
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H -1.907477 1.382186 -0.096845
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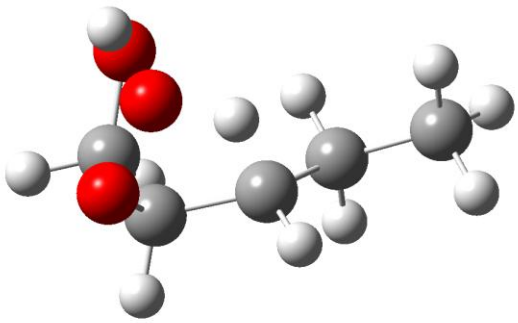

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H 0.108608 -1.031169 0.661532
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H 1.357542 1.270166 0.372816
H 1.934544 0.910220 -1.242903
C 2.995572 -0.146829 0.305541
H 2.807993 -0.585113 1.285934
H 3.772744 0.606987 0.417385
H 3.377427 -0.933634 -0.345667
H -0.907425 -0.230865 -1.974185
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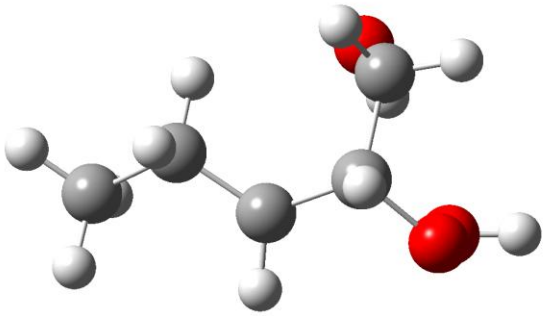
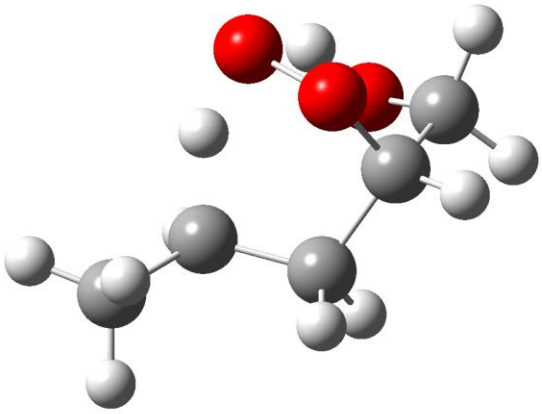
H 0.961601 -1.482362 -0.921113

1,4 inner P



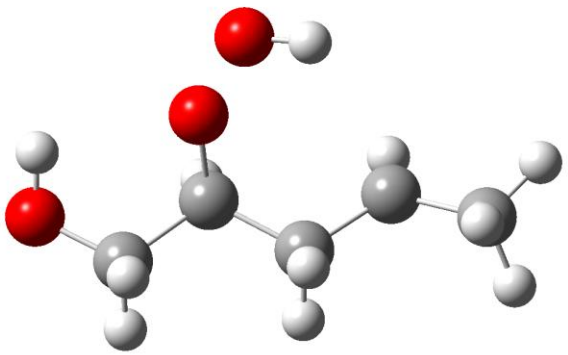
C 0.918005 1.271964 0.549363
H 1.962992 1.443267 0.829477
H 0.294354 1.902066 1.185135
C 0.590919 -0.193377 0.838868
H 0.603408 -0.316667 1.932760
C -0.702948 -0.648959 0.263825
C -1.935455 0.176725 0.362435
H -1.707867 1.202533 0.061481
H -2.266097 0.236549 1.409983
C -3.072105 -0.373900 -0.491902
H -3.323627 -1.392068 -0.193181
H -3.968964 0.236764 -0.399512
O 0.668394 1.667028 -0.779950
H 1.005403 0.971721 -1.353236
O 1.658352 -1.064936 0.468323
O 1.843575 -0.934849 -0.948481
H -2.781020 -0.394945 -1.542044
H 2.806450 -0.923291 -0.994580
H -0.778108 -1.698597 0.009047

1,5 TS



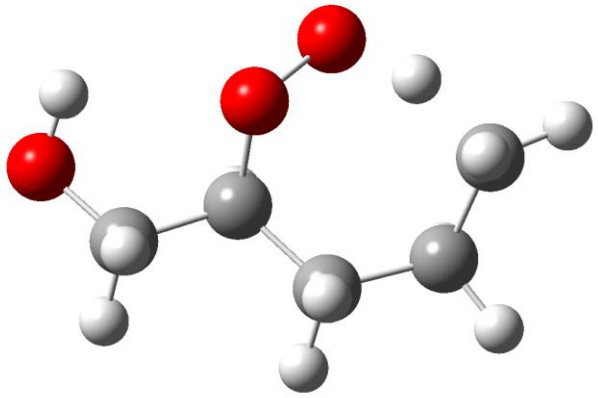
C -0.742732 0.236663 -0.940585
H -1.039269 0.488833 -1.960429
C 0.510176 -0.670687 -0.966254
H 1.124734 -0.360886 -1.811818
H 0.174641 -1.695494 -1.140453
C 1.327026 -0.589118 0.302604
H 0.739868 0.446551 0.886155
O -0.371524 1.491929 -0.389528
O -0.104116 1.310781 0.961743
C -1.938518 -0.391341 -0.237138
H -2.374253 -1.130380 -0.910572
H -2.683470 0.390988 -0.062363
C 2.775609 -0.211852 0.155207
H 3.315815 -0.984039 -0.402558
H 3.263978 -0.095408 1.120953
H 2.874783 0.722173 -0.399746
O -1.624564 -1.080232 0.952785
H -1.305541 -0.423321 1.579308
H 1.120974 -1.380830 1.018529

1,5 P



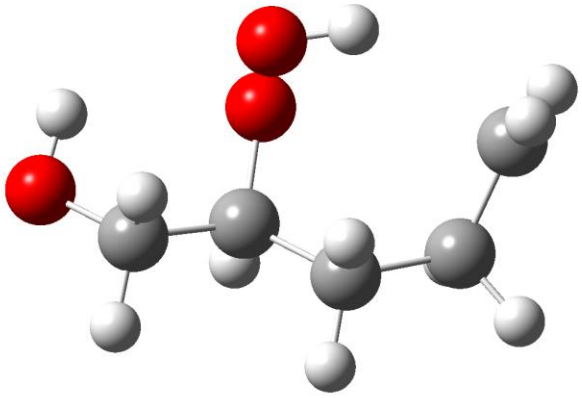
C	-1.761253	-1.049683	0.144208
H	-1.728755	-1.994575	-0.397497
C	-0.571783	-0.197687	-0.261984
C	0.754946	-0.893432	0.009909
H	0.739280	-1.858078	-0.521020
C	1.957659	-0.113203	-0.395032
H	1.920839	0.400504	-1.348496
C	3.286380	-0.432483	0.191068
H	3.671065	-1.389108	-0.187056
H	3.224210	-0.530828	1.276824
H	4.029951	0.327019	-0.045304
O	-2.982860	-0.428671	-0.171398
H	-0.667070	0.084015	-1.313781
O	-0.713022	0.986296	0.522280
O	-0.077377	2.070457	-0.132512
H	0.834457	1.994561	0.183831
H	-2.951876	0.465320	0.183886
H	-1.691400	-1.268866	1.216547
H	0.809685	-1.135696	1.076088

1,6 TS



C -0.533460 -0.283898 -0.250744
C 0.545066 -1.289633 0.120400
C 1.956301 -0.930699 -0.354636
H 1.952128 -0.789237 -1.438010
C 2.516325 0.296537 0.310398
H 3.450138 0.679810 -0.089971
O -0.329744 0.978718 0.395265
O 0.598992 1.729761 -0.303840
H 0.543993 -1.410284 1.207585
H 2.620409 -1.779043 -0.158115
H 1.626481 1.244407 0.010466
H 0.260955 -2.252715 -0.309714
H -0.554590 -0.100335 -1.328486
C -1.908985 -0.719141 0.219873
H -2.148839 -1.687517 -0.218069
H -1.891820 -0.832891 1.310337
O -2.911900 0.181074 -0.184108
H -2.637319 1.062863 0.086479
H 2.468209 0.309525 1.397216

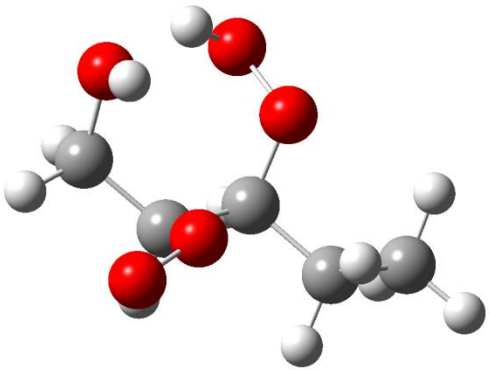
1,6 P



C -0.454073 -0.488376 -0.315921
H -0.567217 -0.951663 -1.300666
C -1.755209 -0.643372 0.452603
H -1.964891 -1.703790 0.595184
H -1.648288 -0.179289 1.437660
C 0.735048 -1.097725 0.410007
H 0.552824 -2.171913 0.476206
H 0.775478 -0.721606 1.434951
C 2.075170 -0.840726 -0.296148
H 1.939902 -0.928940 -1.375321
H 2.770032 -1.638211 -0.005793
C 2.688044 0.474069 0.036477
H 0.826382 1.789418 0.541163
H 2.898922 0.710952 1.071711
H 3.152348 1.086360 -0.721282
O -2.841583 -0.094903 -0.255646
H -2.592613 0.797174 -0.518264
O -0.260916 0.879136 -0.676427
O -0.132096 1.651804 0.512366

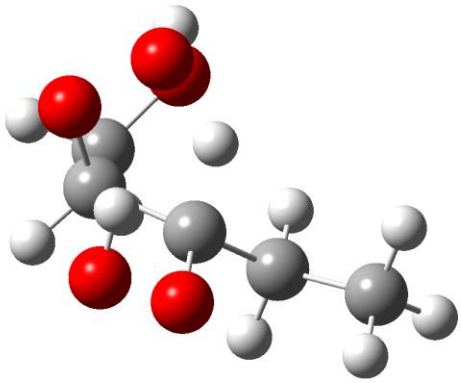
M06-2X/aug-cc-pVTZ calculated geometry coordinates for H-shift reaction in the ROO_3OOH <-> ROOH_3OO cycle.

ROO_3OOH



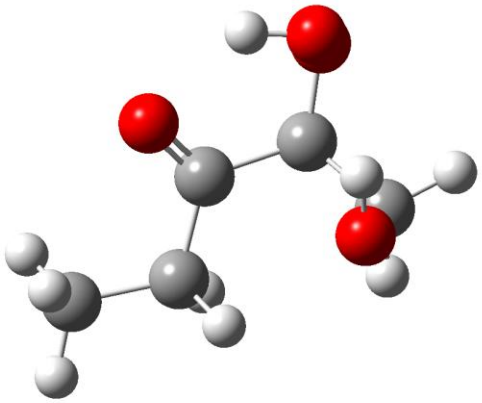
H	2.6255070	-0.0736350	1.1383360
C	1.7380420	0.4882580	0.8424810
H	1.4616560	1.1612900	1.6533010
C	0.6039150	-0.4992190	0.6088220
C	-0.7964030	0.0642270	0.3824690
C	-1.7990490	-1.0227370	0.0147350
H	-1.6524180	-1.8690140	0.6892940
H	-1.5676660	-1.3769140	-0.9904470
C	-3.2342780	-0.5215740	0.0866050
H	-3.3707230	0.3368030	-0.5684910
H	-3.4909510	-0.2175560	1.1021440
H	-3.9323740	-1.2994580	-0.2181640
O	2.0254310	1.2967990	-0.2843480
H	2.2218360	0.7295330	-1.0367400
H	0.5670270	-1.1874240	1.4562070
O	0.9407800	-1.2980400	-0.5588550
O	1.9556020	-2.0766830	-0.3317920
H	-1.1011810	0.5529780	1.3135610
O	-0.8536610	1.0223300	-0.6570710
O	-0.4806950	2.2907780	-0.1409110
H	0.4662760	2.3082000	-0.3658530

1,4 in ROO_3OOH TS



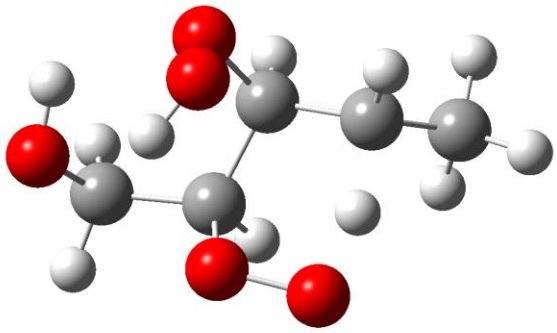
C 0.809253 0.394846 -0.688209
C -0.572762 0.000785 -0.117189
O 1.341550 1.292428 0.284200
O 0.999182 0.750499 1.529504
H -0.121609 0.213071 1.076234
O -1.591219 0.877484 -0.396757
O -1.160522 2.223584 -0.374053
H -0.786126 2.333709 0.515595
C -1.100729 -1.399701 -0.282773
H -0.309800 -2.085880 0.012357
H -1.300548 -1.562376 -1.347361
C -2.365231 -1.656447 0.532053
H -2.181015 -1.471718 1.590683
H -2.679046 -2.692350 0.419896
H -3.182190 -1.013607 0.212783
H 0.698261 0.979144 -1.603924
C 1.746315 -0.777826 -0.928882
H 2.678997 -0.368045 -1.328949
H 1.317712 -1.436614 -1.686442
O 1.990977 -1.556682 0.217477
H 2.124542 -0.963775 0.966164

1,4 in ROO_3OOH P



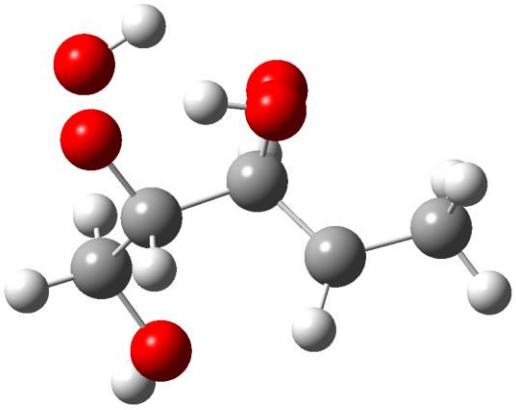
C 1.075714 1.444710 0.377648
H 2.097405 1.614489 0.727992
H 0.433270 2.206458 0.820083
C 0.638782 0.065018 0.868650
H 0.458638 0.113110 1.947358
C -0.652955 -0.385423 0.187274
C -1.834791 0.541423 0.299988
H -1.574727 1.428755 -0.285629
H -1.914121 0.877745 1.337593
C -3.127201 -0.083057 -0.195231
H -3.374246 -0.973837 0.379960
H -3.949452 0.624521 -0.110460
O 0.968896 1.587837 -1.019804
H 1.516572 0.902524 -1.417727
O 1.651644 -0.909109 0.752791
O 2.003014 -1.035080 -0.622155
H -3.030411 -0.382096 -1.236581
H 1.301344 -1.633658 -0.927895
O -0.693749 -1.427903 -0.418915

1,5 in ROO_3OOH TS



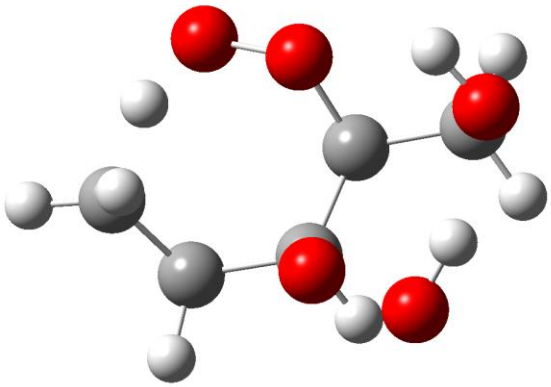
C -0.331756 -0.816869 -0.514952
H 0.227284 -1.541430 -1.117514
C 0.381952 0.552062 -0.628942
C 1.730770 0.528381 0.037065
H 1.524132 -0.458311 0.911584
O -0.317469 -1.236443 0.836588
O 0.993596 -1.497859 1.198731
H 0.484924 0.770513 -1.698931
H 1.914245 1.403541 0.653442
C 2.878563 0.049552 -0.808184
H 2.654849 -0.912703 -1.271336
H 3.785716 -0.064281 -0.218007
H 3.088371 0.764713 -1.609254
O -0.436030 1.620171 -0.166496
O -0.536948 1.554590 1.249204
H -1.152375 0.813807 1.387416
C -1.785650 -0.808565 -0.964930
H -2.174914 -1.821499 -0.875938
H -1.820328 -0.522691 -2.021079
O -2.621996 0.010964 -0.177242
H -2.424401 0.929587 -0.387014

1,5 in ROO_3OOH P



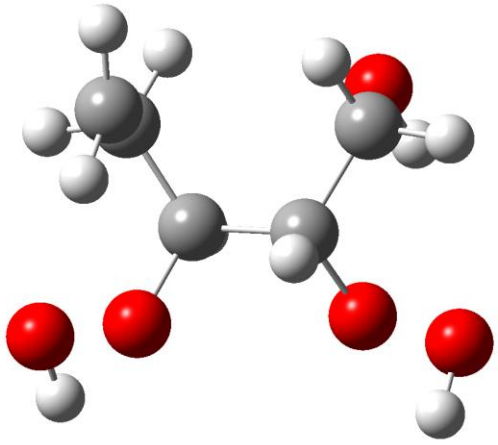
C -1.817387 1.157657 -0.002165
H -2.080638 0.961180 1.039824
H -2.721884 1.087386 -0.611711
C -0.834119 0.101045 -0.475934
H -0.610896 0.264676 -1.533053
C 0.477626 0.093122 0.328008
C 1.507781 1.013064 -0.204542
H -0.903184 -1.942615 1.140702
O -1.183797 2.415834 -0.150376
H -1.759476 3.103608 0.188871
O -1.446027 -1.180302 -0.476476
O -1.745847 -1.548905 0.864263
H 0.261978 0.322809 1.380882
O 0.971278 -1.254513 0.452158
O 1.301721 -1.740415 -0.841663
H 0.449656 -2.096147 -1.136275
H 1.274140 1.627111 -1.059851
C 2.869138 1.000326 0.383924
H 3.429732 0.118869 0.053308
H 3.437746 1.884432 0.103279
H 2.825963 0.943816 1.475018

1,6 in ROO_3OOH TS



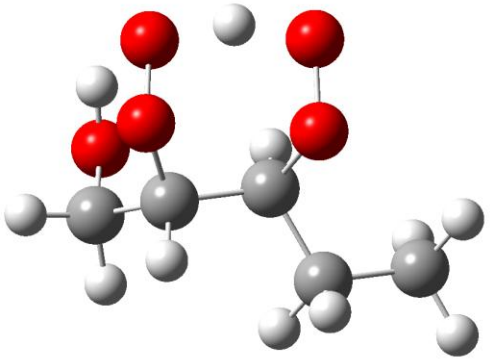
C 0.198651 -0.705951 0.692976
H -0.217414 -1.136730 1.609352
C -0.196964 0.775265 0.647213
C -1.707257 1.023981 0.663203
H -1.853849 2.102811 0.769198
C -2.421397 0.539193 -0.568602
H -1.979174 0.831365 -1.516703
O -0.295294 -1.451598 -0.418135
O -1.630037 -1.767551 -0.240865
H 0.238848 1.248531 1.532174
H -2.132594 0.552131 1.551060
H -2.183512 -0.763043 -0.548047
H -3.504621 0.606320 -0.542915
C 1.696408 -0.985498 0.676681
H 1.854978 -2.032303 0.943576
H 2.201348 -0.354835 1.407091
O 2.293971 -0.717263 -0.583157
H 1.785851 -1.178088 -1.259473
O 0.289896 1.451454 -0.498489
O 1.622591 1.875628 -0.259994
H 2.124478 1.116543 -0.609013

1,6 in ROO_3OOH P



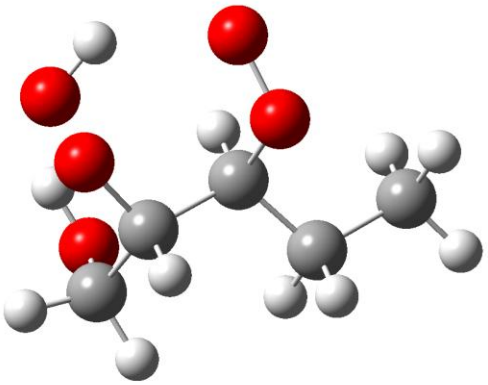
C 1.434851 1.236618 0.173462
H 2.397299 1.140090 0.681036
H 0.898103 2.074285 0.616100
C 0.651600 -0.047085 0.378833
H 0.483193 -0.222132 1.445417
C -0.681395 -0.073950 -0.357382
C -1.493059 1.210436 -0.210126
H -2.433524 1.041156 -0.747981
C -1.762290 1.572814 1.205731
H -1.848208 2.605718 1.505012
O 1.606282 1.520717 -1.199864
H 2.074846 0.778636 -1.594410
O 1.383901 -1.143635 -0.170091
O 2.523956 -1.362787 0.650381
H -0.497346 -0.275134 -1.415778
O -1.370469 -1.184939 0.209273
O -2.511673 -1.444503 -0.595462
H -2.246799 -2.255317 -1.046487
H -0.973875 2.010437 -0.738571
H 2.280510 -2.181562 1.099360
H -2.088410 0.811997 1.899290

ROO_3OOH <-> ROOH_3OO TS



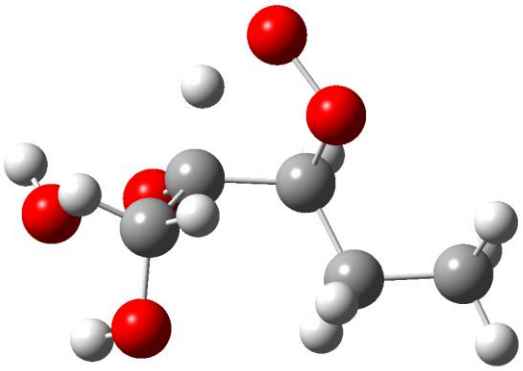
C 0.607086 -0.494150 -0.794414
H 0.343911 -0.750408 -1.823073
C -0.649515 -0.100588 -0.020695
H -0.497637 -0.201864 1.053616
O -0.869920 1.304559 -0.289832
O -0.303109 2.060581 0.680171
O 1.430139 0.677143 -0.985628
O 1.817705 1.196457 0.207246
H 0.815975 1.773907 0.588872
C -1.879261 -0.859889 -0.472244
H -1.640676 -1.926120 -0.446672
H -2.075308 -0.604211 -1.516436
C -3.096280 -0.563448 0.392172
H -2.919559 -0.865917 1.424438
H -3.972527 -1.096662 0.028042
H -3.319480 0.502419 0.385772
C 1.398024 -1.637130 -0.180213
H 2.328351 -1.747919 -0.746446
H 0.826707 -2.560120 -0.294407
O 1.643673 -1.483254 1.196701
H 2.082014 -0.635765 1.329391

ROOH_3OO



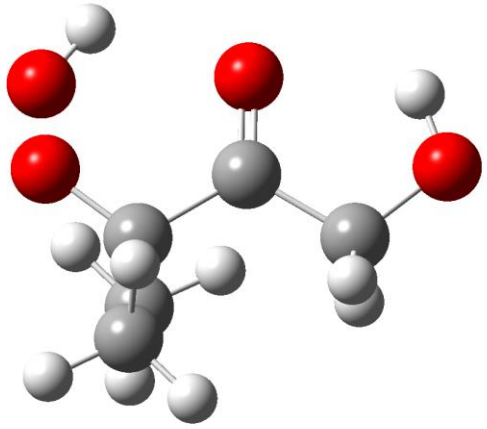
C -1.341077 -1.541345 0.482855
H -2.354111 -1.521806 0.894511
H -0.793839 -2.344715 0.975175
C -0.689556 -0.200603 0.811985
H -0.468618 -0.161658 1.882511
C 0.599846 0.021258 0.024583
C 1.689663 -0.976829 0.357970
H 1.299244 -1.968756 0.129486
H 1.887553 -0.942598 1.432178
C 2.968148 -0.727825 -0.432200
H 3.378448 0.256946 -0.215550
H 3.723610 -1.472191 -0.187526
O -1.344579 -1.841178 -0.894924
H -1.828981 -1.138054 -1.340422
H 2.773717 -0.785431 -1.503548
H 0.398011 0.030037 -1.045137
O 1.110790 1.338278 0.357325
O 0.548832 2.280683 -0.334224
O -1.594579 0.879329 0.654297
O -1.973120 0.962480 -0.715404
H -1.355929 1.643552 -1.029402

1,4 in ROOH_3OO TS



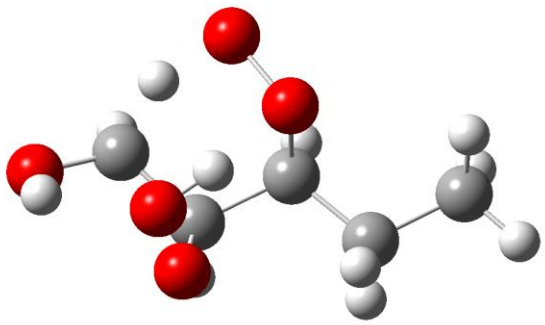
C 0.870327 0.255938 -0.365391
H 1.018679 0.618996 -1.388693
C -0.627061 0.393340 -0.041367
O 1.439341 1.176025 0.552315
O 0.662192 2.324033 0.410275
H -0.425542 1.661068 0.215348
C 1.492416 -1.108597 -0.168384
H 0.936317 -1.816726 -0.784470
H 1.351947 -1.417481 0.868112
C 2.970860 -1.111945 -0.540113
H 3.398349 -2.105419 -0.415733
H 3.529910 -0.418937 0.086622
H 3.110254 -0.812605 -1.579684
C -1.149047 -0.239606 1.228020
H -2.060502 0.264497 1.550125
H -0.390384 -0.097548 1.996447
O -1.353932 -1.628425 1.075395
H -2.106566 -1.757748 0.490676
O -1.344791 0.136543 -1.187277
O -2.727469 -0.001406 -0.885615
H -3.110159 0.692960 -1.436086

1,4 in ROOH_3OO P



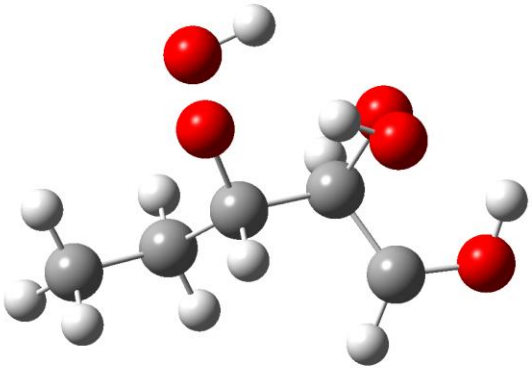
C 1.846435 0.381216 -0.556635
H 1.746328 1.458146 -0.371960
C 0.616266 -0.298734 0.003256
C -0.727686 0.023967 -0.629001
C -1.042959 1.517042 -0.567776
H -2.026760 1.653070 -1.016487
H -0.329948 2.046229 -1.202012
C -1.023426 2.070505 0.852207
H -0.036963 1.968766 1.308927
H -1.282355 3.127643 0.854993
O 3.015623 -0.115390 0.015110
H 2.750225 -0.718252 0.722658
H -1.736254 1.539943 1.480442
H 1.858406 0.242963 -1.643450
H -0.692111 -0.311684 -1.672069
O -1.772193 -0.638006 0.039187
O -1.625866 -2.032341 -0.176299
H -1.015197 -2.267832 0.538413
O 0.726543 -1.077134 0.920532

1,5 in ROOH_3OO TS



C -1.604054 0.538576 -0.825061
H -1.588065 1.116160 -1.747749
C -0.489731 -0.492671 -0.754991
H -0.425710 -1.051258 -1.694092
C 0.855238 0.192239 -0.483818
H 1.056114 0.921051 -1.276911
O 0.719542 0.902708 0.747300
O -0.136261 1.978944 0.550010
H -1.143432 1.405301 0.011913
O -2.867896 0.110683 -0.555238
H -2.836316 -0.447456 0.233519
O -0.761437 -1.504257 0.204184
O -1.226654 -0.918710 1.420047
H -0.463504 -0.398615 1.723430
C 2.010041 -0.775543 -0.322798
H 2.031446 -1.416665 -1.206172
H 1.799966 -1.426081 0.527526
C 3.344766 -0.064008 -0.145953
H 4.151982 -0.784240 -0.025301
H 3.327748 0.578862 0.732201
H 3.573860 0.556441 -1.013070

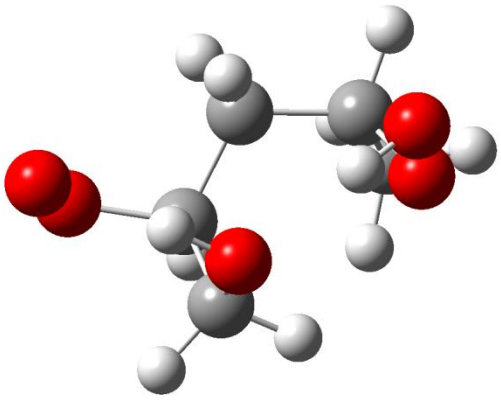
1,5 in ROOH_3OO P



C 1.554951 -1.331804 0.137063
H 1.151345 -2.264004 0.499186
C 0.699566 -0.239556 -0.381943
H 0.554552 -0.322643 -1.469441
C -0.663595 -0.180894 0.317230
C -1.669103 -1.137484 -0.299524
H -1.234210 -2.139785 -0.281259
H -1.802963 -0.867247 -1.347960
C -3.006081 -1.121376 0.427011
H -2.883415 -1.385948 1.478188
H -3.453522 -0.130001 0.379536
O 2.830535 -1.400855 -0.302139
H 3.121800 -0.510187 -0.534762
O 1.388838 1.018347 -0.311107
O 1.601963 1.358763 1.052698
H 0.769502 1.806044 1.268531
H -3.700181 -1.830985 -0.019925
H -0.531650 -0.405149 1.379991
O -1.135712 1.162111 0.358933
O -1.316005 1.626243 -0.971899
H -0.442631 1.999712 -1.162991

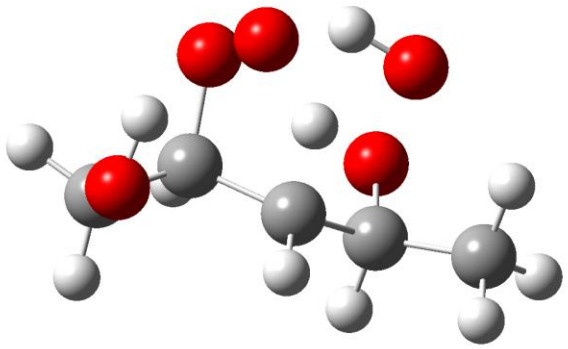
M06-2X/aug-cc-pVTZ calculated geometry coordinates for H-shift reaction in the ROO_4OOH <-> ROOH_4OO cycle.

ROO_4OOH



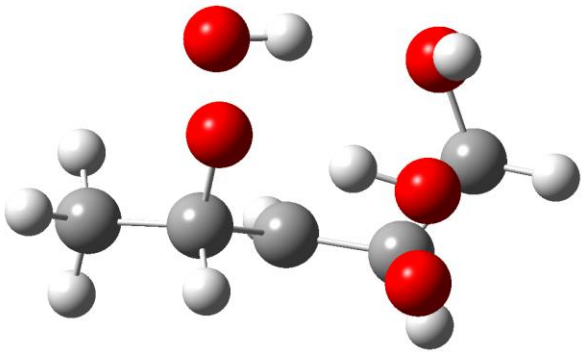
H -0.02651600 0.58710300 1.83799700
C -0.90476300 0.54465900 1.19788100
H -1.79833700 0.50626300 1.82677300
C -0.83342400 -0.73364300 0.37603000
C 0.12047100 -0.70611100 -0.80848900
H -0.16269900 0.11253100 -1.46953200
C 1.59870600 -0.57434500 -0.44330700
H 2.17050700 -0.59943200 -1.37478200
C 2.09809600 -1.65333700 0.50018600
H 1.85715300 -2.64084700 0.10797200
H 1.64491600 -1.54860200 1.48644100
H 3.17637400 -1.57492500 0.61949600
O -0.89257700 1.72723600 0.42084400
H -1.65711000 1.69072300 -0.16508200
H -0.00832700 -1.63412500 -1.36829800
O 1.89397000 0.64597400 0.21921500
O 1.67321400 1.71891400 -0.68328200
H 0.78977500 2.01276200 -0.39677600
H -0.61737100 -1.57123800 1.04004600
O -2.16119800 -1.08188800 -0.12505600
O -2.74376900 -0.08567900 -0.71647800

1,4 in ROO_4OOH TS



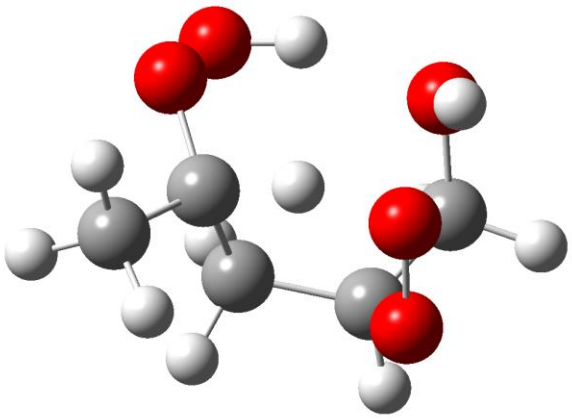
C -0.944759 0.073118 -0.754225
C 0.019482 -0.780389 0.070404
H -0.146319 0.037549 1.091053
H -0.606851 0.216063 -1.782901
O -0.849675 1.373537 -0.150833
O -0.812141 1.107601 1.225571
H -0.377102 -1.732093 0.414353
C 1.455743 -0.839364 -0.374481
H 1.492451 -1.493701 -1.256842
C 2.391123 -1.379731 0.692153
H 2.075555 -2.377449 0.995546
H 2.384712 -0.727732 1.562763
H 3.404804 -1.433163 0.300705
O 1.901507 0.393655 -0.918216
C -2.369697 -0.455506 -0.738092
H -3.020422 0.302567 -1.185259
H -2.415157 -1.350333 -1.360981
O -2.818347 -0.829283 0.542728
H -2.672618 -0.089346 1.141796
O 2.004950 1.345162 0.132178
H 1.159237 1.813492 0.053784

1,4 in ROO_4OOH P



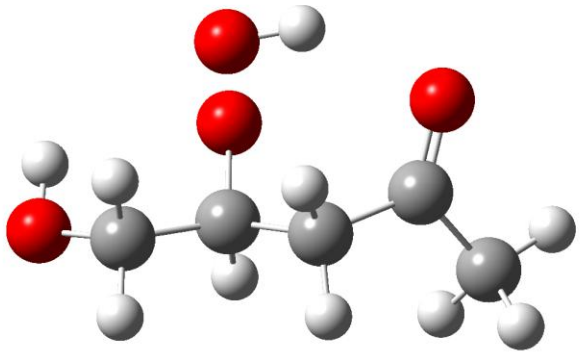
C 1.052022 -0.959120 -0.599755
C -0.386081 -0.721723 -0.935155
H 0.450441 0.100831 1.702507
C -1.456328 -0.606544 0.090033
C -2.847774 -0.546203 -0.503500
H -2.930034 0.302653 -1.179655
H -3.053590 -1.461086 -1.058225
H -3.587736 -0.437286 0.286602
C 1.951036 0.193713 -1.050481
H 2.973115 -0.007819 -0.723080
H 1.935791 0.234050 -2.139222
O 1.517692 1.464118 -0.592008
H 1.744488 1.499469 0.343862
H -1.375825 -1.430095 0.807101
O -1.215182 0.526041 0.958831
O -1.249296 1.721600 0.193414
H -0.357237 1.745381 -0.203535
H 1.402311 -1.851547 -1.134938
O 1.259609 -1.327177 0.760258
O 1.380629 -0.173975 1.587838
H -0.626592 -0.540157 -1.974925

1,5 in ROO_4OOH TS



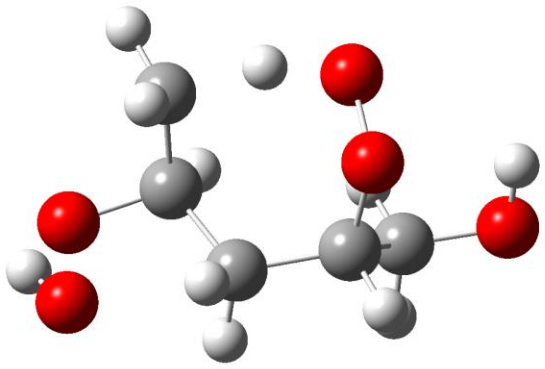
C -1.160980 -0.589198 0.861003
H -1.661048 -1.013137 1.734112
C 0.310471 -0.304686 1.220118
H 0.650469 -1.131580 1.841671
H 0.385721 0.619711 1.790595
C 1.214483 -0.228856 0.001635
H 0.424738 -0.650321 -0.892647
O -1.184467 -1.654523 -0.082941
O -0.698602 -1.193353 -1.301004
C -1.994796 0.605267 0.415764
H -2.042267 1.320324 1.237657
H -3.008178 0.253464 0.207051
C 2.360895 -1.208674 -0.053869
H 3.029567 -1.045170 0.793918
H 2.925192 -1.079989 -0.975245
H 1.971446 -2.224590 -0.013749
O 1.711918 1.017121 -0.356210
O 0.941981 2.102900 0.118874
H 0.080832 1.989717 -0.341127
O -1.489498 1.310499 -0.708277
H -1.387562 0.657302 -1.413692

1,5 in ROO_4OOH P



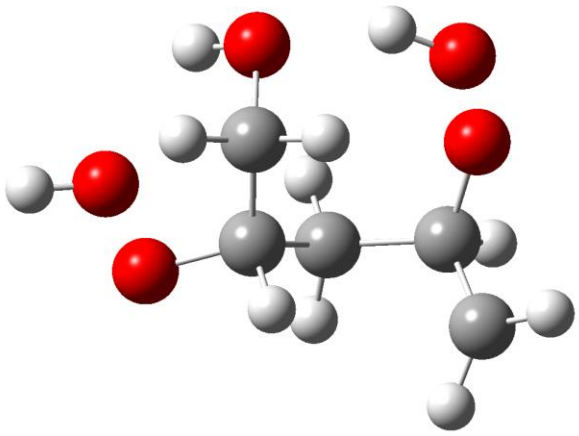
C -1.958184 -0.694843 0.539328
H -1.991310 -1.697288 0.967318
H -2.056002 0.032333 1.350753
C -0.623575 -0.480074 -0.153629
H -0.535939 -1.182953 -0.986348
C 0.553541 -0.634302 0.817011
H 0.653742 -1.687897 1.078056
H 0.355050 -0.059005 1.720574
C 1.822179 -0.108752 0.180666
H 0.315520 1.980007 0.275380
C 2.686952 -1.092527 -0.553835
H 3.492795 -0.578609 -1.068272
H 3.095842 -1.813591 0.156408
H 2.080573 -1.655404 -1.265964
O -3.023370 -0.595196 -0.373178
H -2.943281 0.253493 -0.820762
O 2.097207 1.067553 0.239740
O -0.606948 0.775720 -0.820133
O -0.635948 1.810910 0.155523

1,6 in ROO_4OOH TS



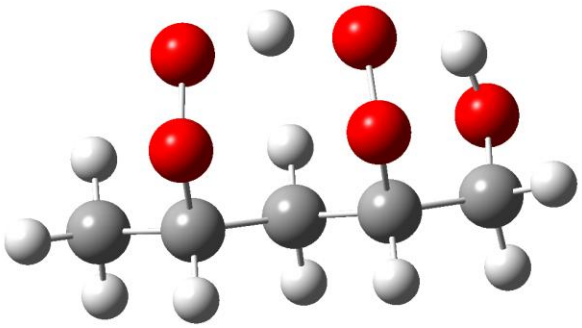
C 1.054970 -0.371106 0.751769
C -0.464109 -0.389081 0.900145
H -0.780374 -1.429916 0.986213
C -1.270433 0.252478 -0.226125
C -1.109947 1.744149 -0.286669
H -1.547212 2.240942 -1.146113
H -0.734175 0.112042 1.831740
H -1.015315 -0.189224 -1.193369
H -1.229491 2.267478 0.658088
H 1.501585 -0.757485 1.669925
O 1.577541 0.964439 0.716393
O 1.346921 1.538434 -0.523325
H 0.237124 1.844273 -0.483519
C 1.583139 -1.192317 -0.413994
H 1.143448 -0.854576 -1.354954
H 1.295690 -2.232397 -0.259017
O 2.988508 -1.155216 -0.472864
H 3.257833 -0.234504 -0.547433
O -2.666625 0.042333 -0.002162
O -2.924635 -1.349993 -0.161915
H -3.464504 -1.351334 -0.961326

1,6 in ROO_4OOH P



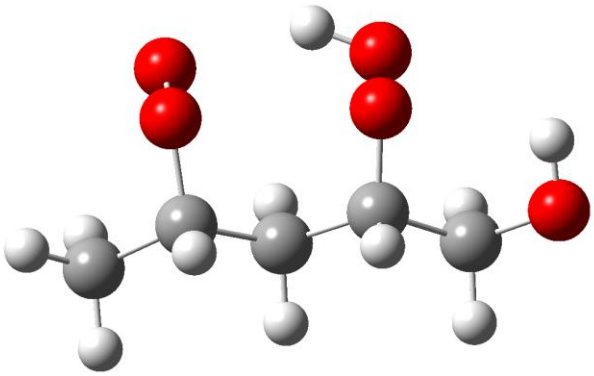
C -0.805306 -0.713301 0.416364
C 0.133908 -0.733757 -0.784046
H -0.040249 -1.665411 -1.325014
C 1.621218 -0.665305 -0.429692
C 2.052687 -1.748100 0.487443
H 1.664537 -2.746657 0.357590
C -0.787094 0.577244 1.227149
H -1.666807 0.586721 1.876597
H 0.107778 0.595888 1.844790
O -0.744622 1.752967 0.431293
H -1.501935 1.720128 -0.162228
H -0.107452 0.082258 -1.462837
H 2.184914 -0.714702 -1.372900
O 1.990044 0.547063 0.218194
O 1.806899 1.618378 -0.693422
H 0.934028 1.944656 -0.407170
H 2.898565 -1.588051 1.137489
H -0.562035 -1.536473 1.094081
O -2.130523 -1.060094 0.017224
O -2.626203 0.024913 -0.784285
H -3.568577 -0.044868 -0.595737

ROO_4OOH <-> ROOH_4OO TS



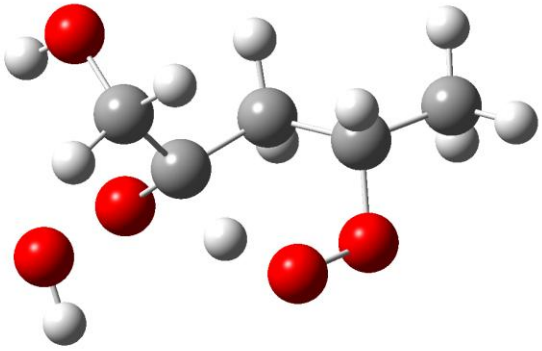
C -0.956886 -0.408030 -0.792374
H -0.864852 -0.708824 -1.838701
C 0.151017 -1.024098 0.046134
H 0.048733 -2.109895 0.002415
H 0.026685 -0.742272 1.090465
C 1.546168 -0.648785 -0.430235
O 1.698981 0.781816 -0.507775
O 1.471181 1.359231 0.693378
O -0.817892 1.020636 -0.881705
O -0.842136 1.588603 0.349856
H 1.683144 -0.939703 -1.473850
H 0.326615 1.594235 0.648044
C 2.636813 -1.241181 0.441305
H 2.523894 -0.885356 1.463865
H 3.617662 -0.948376 0.072209
H 2.568563 -2.328289 0.436953
C -2.354821 -0.770757 -0.299144
H -2.525726 -1.829501 -0.499311
H -3.080825 -0.192621 -0.879340
O -2.532545 -0.584480 1.082602
H -2.278347 0.321265 1.292281

ROOH_4OO



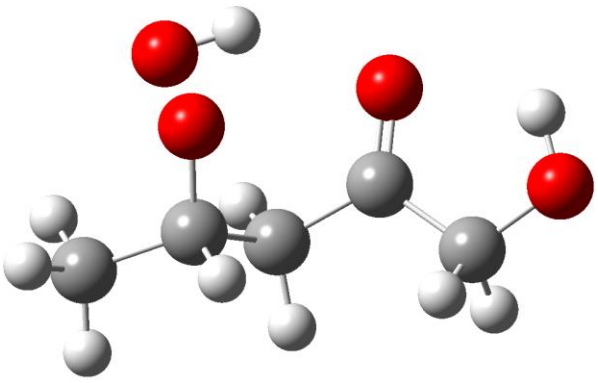
C 2.183806 -0.886052 -0.453099
H 2.230112 -1.971836 -0.541576
H 2.113035 -0.461812 -1.459228
C 0.945620 -0.498969 0.341646
H 1.006959 -0.952853 1.335168
C -0.336500 -0.913629 -0.361455
H -0.280452 -1.984388 -0.569598
H -0.417528 -0.406987 -1.324379
C -1.608066 -0.674709 0.432185
O 3.359332 -0.471951 0.197559
H 3.263506 0.463909 0.402608
O -1.818830 0.756816 0.656173
O -1.891171 1.423549 -0.450590
O 0.984168 0.890172 0.660379
O 0.979966 1.635256 -0.550802
H -1.503100 -1.041581 1.453889
C -2.843443 -1.245750 -0.231104
H -2.753404 -2.328492 -0.303805
H -3.734725 -1.006761 0.346153
H -2.949737 -0.832947 -1.233120
H 0.069098 1.967661 -0.576895

1,5 in ROOH_4OO TS



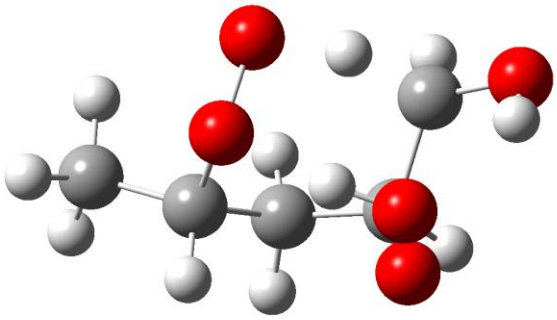
C -0.645061 -0.040969 -0.047818
H -0.036171 -1.009215 0.615800
C 0.543344 0.667019 -0.646454
H 0.368796 1.746069 -0.648545
H 0.675399 0.335009 -1.677141
C 1.830975 0.354001 0.131539
O 1.932069 -1.058690 0.249221
O 0.959691 -1.486383 1.137693
H 1.773633 0.771706 1.140636
C 3.072067 0.830394 -0.586991
H 3.961740 0.597063 -0.005942
H 3.022982 1.907636 -0.739333
H 3.151222 0.345491 -1.559750
C -1.432131 0.712840 1.001783
H -2.123451 0.044441 1.514972
H -0.729105 1.108240 1.734257
O -2.107905 1.817426 0.434218
H -2.773350 1.483095 -0.174589
O -1.411836 -0.554495 -1.089855
O -2.529491 -1.254803 -0.562821
H -2.247076 -2.173689 -0.660357

1,5 in ROOH_4OO P



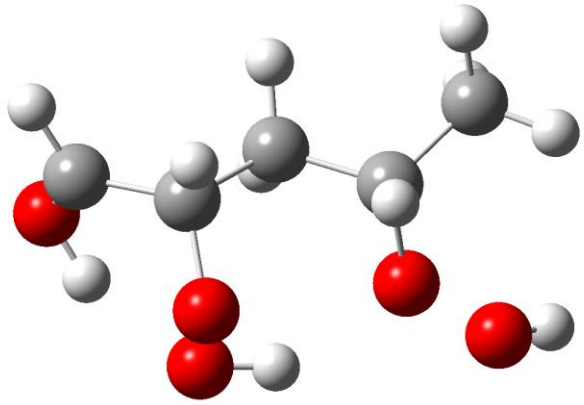
C 2.148671 -0.841352 0.131326
H 1.775284 -1.400797 0.999540
H 2.420877 -1.584862 -0.628574
C 1.002046 -0.029674 -0.414743
H -0.778486 1.886973 -0.403264
C -0.275100 -0.746978 -0.754355
H -0.085802 -1.804710 -0.939813
H -0.693595 -0.299278 -1.655250
C -1.299855 -0.623665 0.388910
O 3.241797 -0.053152 0.473764
H 3.002682 0.861351 0.269671
O -1.334483 0.691571 0.916512
O -1.664439 1.594014 -0.130745
O 1.122858 1.169261 -0.539405
H -0.955204 -1.202354 1.250035
C -2.672043 -1.097563 -0.048395
H -2.624993 -2.125149 -0.408809
H -3.366216 -1.049139 0.788244
H -3.042730 -0.460192 -0.849250

1,6 in ROO_4OO TS



C -1.617422 -0.441364 0.136718
H -1.643810 -1.345222 0.748364
C -0.745197 -0.690603 -1.091853
C 0.766867 -0.700062 -0.834537
H 1.261855 -1.251023 -1.640220
C 1.321175 0.716523 -0.844045
H 1.189020 1.182795 -1.820096
O -1.013067 0.501212 1.040861
O -0.668016 1.663150 0.375568
H -1.048157 -1.649005 -1.513377
H 0.454777 1.364409 -0.150615
H -0.956587 0.070482 -1.847153
C -3.017021 0.001065 -0.232199
H -3.472081 -0.718082 -0.913245
H -2.974457 0.970779 -0.726958
H -3.639124 0.085149 0.656664
O 2.600067 0.888312 -0.413390
H 2.690179 0.414927 0.426652
O 1.122538 -1.452684 0.328602
O 1.381383 -0.624644 1.458201
H 0.504731 -0.241325 1.656749

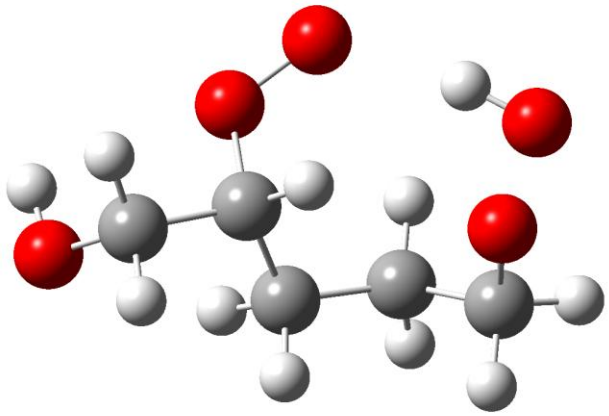
1,6 in ROO_4OO P



C -2.547601 0.698485 0.258677
H 3.325770 -1.169413 -0.656223
C -1.173106 0.425718 0.757929
C -0.076569 1.036459 -0.128019
H -0.152072 2.121126 -0.042871
H -0.259006 0.797394 -1.178222
C 1.338931 0.605212 0.236518
O -2.918158 0.242821 -0.961914
H -2.423424 -0.570269 -1.136860
O 1.541487 -0.626330 -0.474865
O 2.686129 -1.273315 0.058777
H 1.406381 0.373563 1.302302
C 2.388101 1.621955 -0.164315
H 2.256697 2.540496 0.406648
H 3.389704 1.244048 0.034937
H 2.297588 1.857759 -1.225482
H -1.086921 0.837780 1.765957
O -0.938999 -0.968740 0.991650
O -1.014734 -1.655954 -0.253672
H -0.076495 -1.668172 -0.509319
H -3.102552 1.560855 0.594584

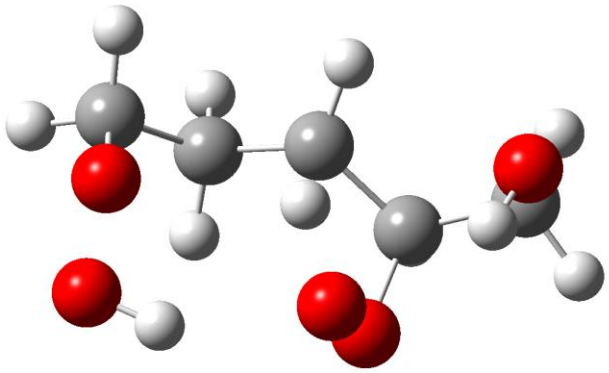
M06-2X/aug-cc-pVTZ calculated geometry coordinates for H-shift reaction in the ROO_5OOH <-> ROOH_5OO cycle.

ROO_5OOH



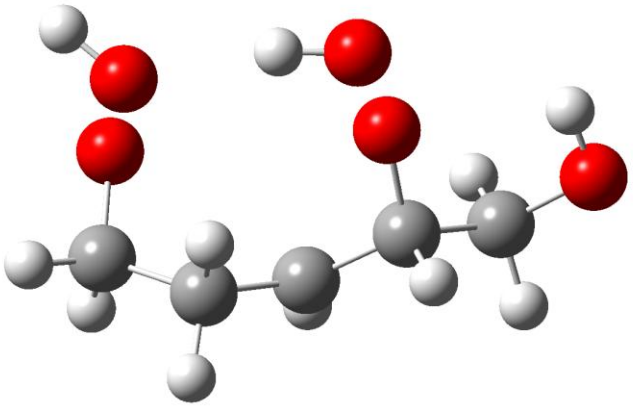
H -2.564144 0.738569 1.495089
C -2.263654 -0.167202 0.961355
H -2.195464 -0.978929 1.685156
C -0.888205 0.045499 0.352456
H -0.176188 0.348120 1.118840
C -0.396113 -1.146304 -0.454894
H -1.126094 -1.329882 -1.243293
C 1.005185 -1.011053 -1.047553
H 1.136866 -1.784298 -1.806770
C 2.129330 -1.175674 -0.037933
H 2.017917 -2.114664 0.510055
H 3.101845 -1.171570 -0.533948
O -3.232592 -0.546694 0.010106
H -3.409730 0.199605 -0.568783
O -1.049486 1.186800 -0.543894
O -0.006829 1.951313 -0.609956
H -0.432181 -2.014615 0.209522
H 1.116130 -0.057204 -1.567194
O 2.130971 -0.190999 0.981325
O 2.568148 1.029439 0.400838
H 1.730091 1.454398 0.153393

1,4 in ROO_5OOH TS



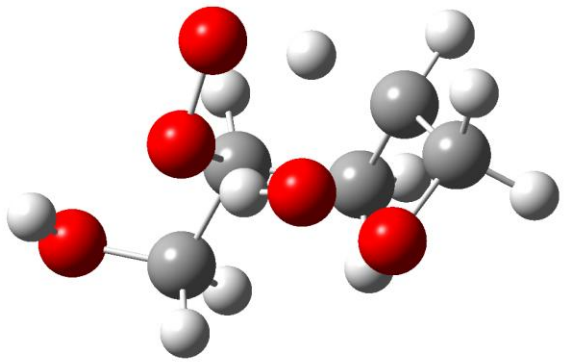
C 1.344469 0.393169 -0.766454
C 0.211275 0.923053 0.108921
H 0.054015 -0.276878 0.580166
H 1.418887 0.903967 -1.730769
O 0.894313 -0.929354 -1.085662
O 0.428031 -1.428193 0.141073
H 0.494026 1.558525 0.944006
C -1.076786 1.250621 -0.589960
H -1.066550 2.296360 -0.915994
H -1.172098 0.632866 -1.483617
C -2.297709 1.034402 0.296970
H -2.272457 1.685214 1.173011
H -3.214581 1.226762 -0.263856
O -2.340255 -0.264293 0.853166
O -2.479116 -1.188731 -0.218904
H -1.595407 -1.592479 -0.239050
C 2.700194 0.403487 -0.079114
H 3.070421 1.429800 -0.058218
H 3.392014 -0.193787 -0.681498
O 2.664360 -0.037627 1.257513
H 2.264400 -0.913155 1.276153

1,4 in ROO_5OOH P



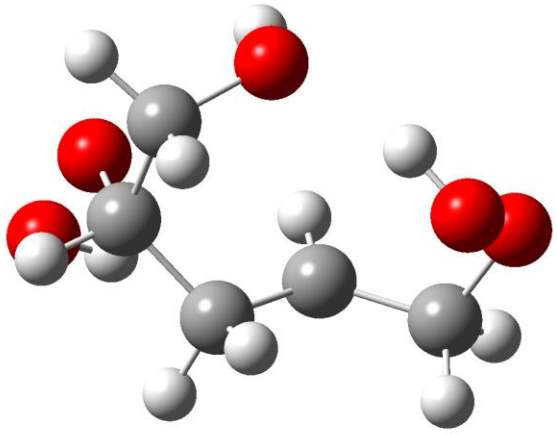
C 1.222242 -0.570262 0.370959
C -0.014287 -1.199305 -0.159087
H -0.010532 -1.616896 -1.158296
C -1.253142 -1.268650 0.660469
C -2.506275 -0.930107 -0.135236
H -2.647972 -1.630949 -0.959969
O 0.987269 0.756350 0.869637
O 0.617863 1.594983 -0.220016
H -0.349681 1.612363 -0.138473
H -1.399832 -2.274836 1.074670
O -2.414181 0.319059 -0.802232
O -2.233840 1.316214 0.203182
H -2.972614 1.909012 0.020929
H -3.393343 -0.942758 0.502249
H -1.169742 -0.589720 1.510149
H 1.563365 -1.069476 1.287279
C 2.359220 -0.560000 -0.636881
H 2.636310 -1.588738 -0.869335
H 2.015350 -0.077925 -1.556665
O 3.500722 0.077024 -0.118217
H 3.219475 0.930828 0.227301

1,5 in ROO_5OOH TS



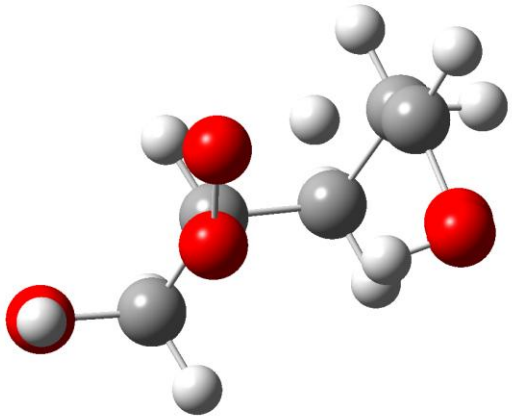
C 1.183398 0.959005 0.838373
H 0.806219 -0.223095 1.329464
C -0.056836 1.364780 0.076207
H 0.158121 1.344181 -0.993860
H -0.368047 2.375042 0.348907
C -1.243762 0.419181 0.335230
O -0.753064 -0.918459 0.334011
O -0.009346 -1.097064 1.490064
H 1.371494 1.503922 1.761013
H -1.693649 0.603339 1.312736
C 2.423912 0.724154 0.012966
H 2.781190 1.675383 -0.398181
H 3.225429 0.279291 0.604936
O 2.179596 -0.065141 -1.131334
C -2.294697 0.480164 -0.751430
H -1.843177 0.159248 -1.697257
H -2.624280 1.512345 -0.868470
O -3.432457 -0.283860 -0.434845
H -3.155557 -1.191954 -0.282606
O 2.039064 -1.412824 -0.706841
H 1.079813 -1.502618 -0.593195

1,5 in ROO_5OOH P



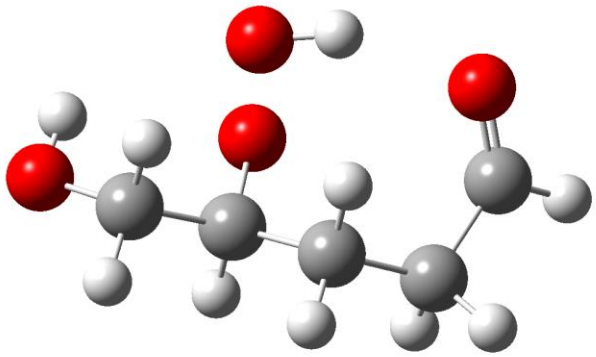
C -0.898116 1.742101 0.346866
H -1.735445 2.400340 0.103240
C -1.434134 0.350485 0.637335
C -0.364185 -0.678876 1.011128
H -0.874826 -1.524969 1.487269
C 0.465963 -1.154466 -0.129349
H -2.184215 -1.875237 -0.748545
C 1.926257 -1.399793 -0.005845
H 2.213348 -1.571785 1.034716
O 0.068606 1.773191 -0.689479
H -2.160529 0.434653 1.451333
O -2.129329 -0.005908 -0.552595
O -2.788166 -1.242150 -0.337319
H -0.310516 1.379461 -1.481091
H -0.405723 2.123605 1.240535
H 0.279968 -0.244218 1.779347
H 0.020880 -1.237234 -1.113375
O 2.708952 -0.324810 -0.523818
O 2.510781 0.794641 0.329169
H 1.771011 1.250099 -0.111645
H 2.244579 -2.251144 -0.610254

1,6 in ROO_5OOH TS



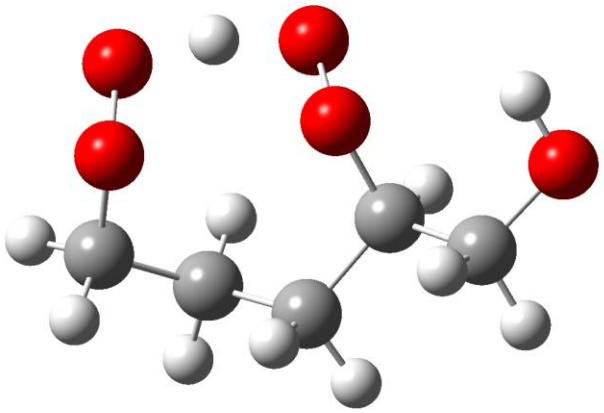
C -1.214157 0.380215 0.208936
C -0.296840 1.483188 -0.299103
C 1.005484 1.675204 0.488964
H 0.785142 1.933067 1.526648
C 1.874116 0.446622 0.506958
H 2.776655 0.470122 1.119336
O -0.603057 -0.914534 0.091389
O 0.153331 -1.193575 1.214267
H -0.061594 1.278804 -1.344989
H 1.564784 2.511490 0.061115
H 1.130997 -0.466325 1.053283
H -0.855864 2.420530 -0.270456
H -1.473296 0.518720 1.261743
O 2.104462 0.006563 -0.775393
O 2.810992 -1.218873 -0.707265
H 2.083683 -1.854364 -0.619675
C -2.482095 0.272697 -0.618337
H -3.006234 1.227706 -0.600306
H -2.210361 0.052841 -1.657458
O -3.363473 -0.695120 -0.104015
H -2.871000 -1.515827 -0.005618

1,6 in ROO_5OOH P



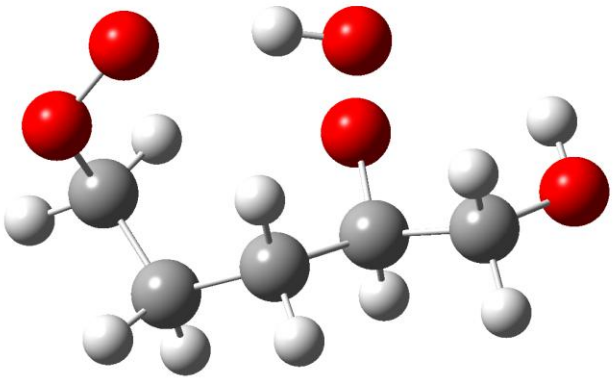
C -2.034377 -0.564365 0.484431
H -2.339892 -1.594116 0.672843
C -0.721096 -0.570747 -0.281383
C 0.421803 -1.170761 0.524232
H 0.131654 -2.180532 0.817559
C 1.728893 -1.225678 -0.254422
H 1.566956 -1.511505 -1.298406
C 2.538574 0.037607 -0.258885
H 3.432860 0.017200 -0.906452
O -3.061348 0.043666 -0.259191
H -0.858221 -1.128581 -1.212945
O -0.414241 0.731560 -0.770717
O -0.387003 1.639785 0.323814
H 0.560803 1.643411 0.546147
H -2.750565 0.916298 -0.521491
H -1.891828 -0.067393 1.447989
H 0.561309 -0.599986 1.444287
H 2.402235 -1.989924 0.149669
O 2.310329 1.017338 0.403214

ROO_5OOH <-> ROOH_5OO TS



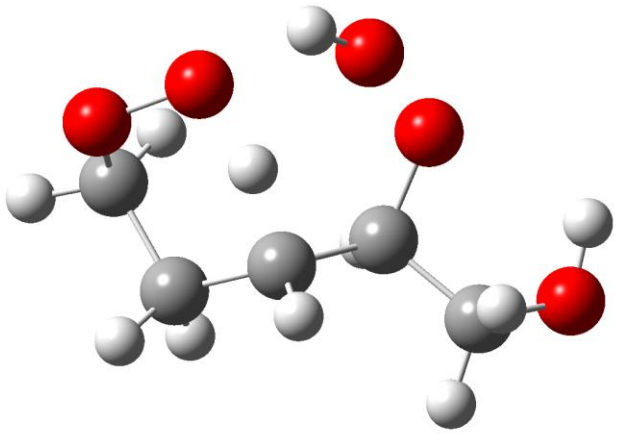
C -2.301176 0.872509 -0.292412
C 1.101890 0.377843 0.304977
H -3.285946 0.812994 0.171853
H 1.255037 0.176906 1.366106
H -2.345440 1.533608 -1.158599
C -1.254205 1.344269 0.699346
H -1.218668 0.654211 1.544141
H -1.616867 2.296270 1.089857
C 0.142231 1.536007 0.095265
H 0.062058 1.740590 -0.976139
H 0.616868 2.409163 0.547093
O 0.061591 -1.652827 0.666122
O 0.608770 -0.845562 -0.275289
O -2.184389 -1.361315 0.083660
O -2.005254 -0.405135 -0.856678
H -1.086772 -1.650403 0.391450
C 2.439575 0.609565 -0.374490
H 2.869141 1.541378 -0.007569
H 2.276514 0.711707 -1.453739
O 3.361263 -0.412253 -0.088032
H 2.968340 -1.250844 -0.348835

ROOH_5OO



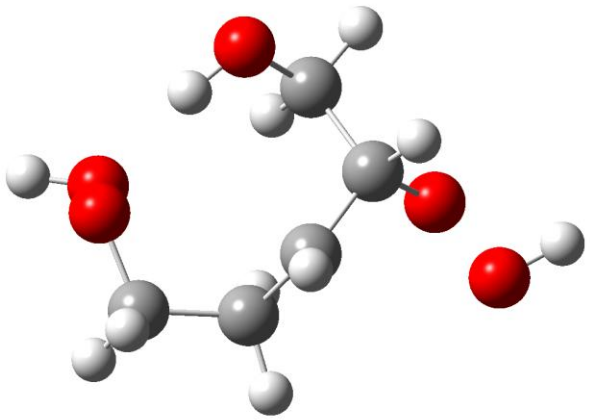
C -2.133916 0.450947 0.767998
C 1.085320 0.618807 0.188472
H -1.547614 -0.243421 1.363893
H 1.301005 1.338384 0.984219
H -2.951388 0.863570 1.356783
C -1.300271 1.558274 0.146214
H -0.978164 2.210220 0.962280
H -1.958519 2.153974 -0.488274
C -0.083968 1.099622 -0.657244
H -0.363591 0.318133 -1.367693
H 0.268677 1.940894 -1.257752
O 0.650541 -1.657103 0.051356
O 0.778194 -0.555087 0.942736
O -2.119408 -1.341102 -0.659599
O -2.800492 -0.311620 -0.268412
H -0.307278 -1.679026 -0.118239
C 2.345351 0.404415 -0.637002
H 2.684439 1.367189 -1.019974
H 2.117113 -0.241388 -1.489777
O 3.390902 -0.122632 0.140949
H 3.062327 -0.920565 0.567646

1,5 in ROOH_5OO TS



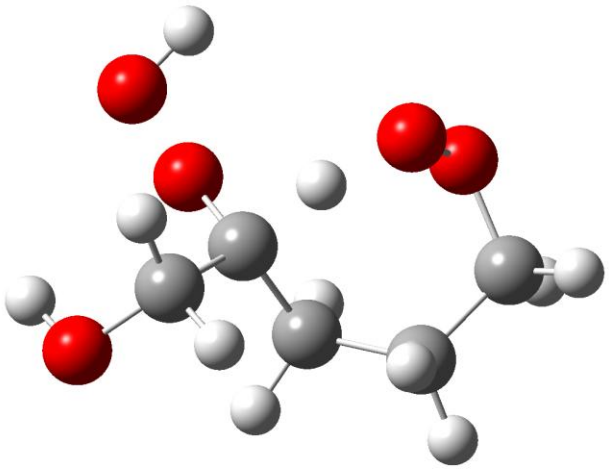
C 2.221333 -0.481715 0.852018
C -1.009295 -0.225086 0.109228
H 3.047755 -0.937313 1.393939
C 1.207602 -1.536355 0.372941
H 0.730754 -1.969735 1.258065
H 1.752062 -2.325551 -0.141916
C 0.188002 -0.902719 -0.531355
H 0.934360 0.094952 -1.016679
H -0.044691 -1.456486 -1.439371
O -0.281616 1.901265 0.666481
O -1.114489 1.160588 -0.211236
O 1.840393 0.886292 -0.919341
H 0.552279 1.937035 0.168362
C -2.317135 -0.819583 -0.392959
H -2.319283 -1.893018 -0.203442
H -2.375170 -0.664562 -1.477423
O -3.427163 -0.272175 0.268208
H -3.349351 0.686400 0.221829
H -0.968316 -0.304316 1.198779
H 1.738951 0.279489 1.468981
O 2.802577 0.117261 -0.290407

1,5 in ROOH_5OO P



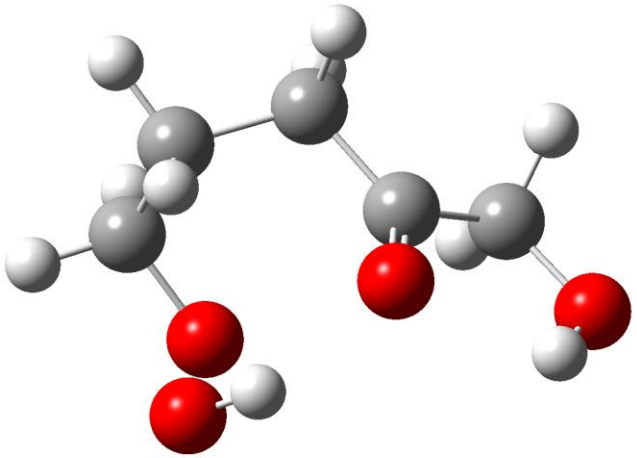
C -1.822645 -1.412882 0.350943
C 1.330659 0.467806 0.367972
H -1.973300 -1.673376 1.400289
C -0.345874 -1.476864 -0.020190
H -0.219362 -1.163222 -1.057066
H -0.042818 -2.528750 0.026379
C 0.496091 -0.648759 0.884672
H -3.311450 0.396625 -1.259728
H 0.494461 -0.861918 1.944437
O 3.034453 -0.969565 -0.232760
O 2.165196 0.048965 -0.714231
O -2.366800 0.267976 -1.111821
H 3.882536 -0.510192 -0.226981
C 0.497198 1.601821 -0.248790
H -0.026113 1.222110 -1.130832
H 1.167723 2.399216 -0.566913
O -0.396913 2.145982 0.689885
H -1.134073 1.531117 0.783296
H 1.951656 0.877569 1.168716
H -2.424809 -2.075257 -0.274185
O -2.348062 -0.093439 0.267046

1,6 in ROOH_5OO TS



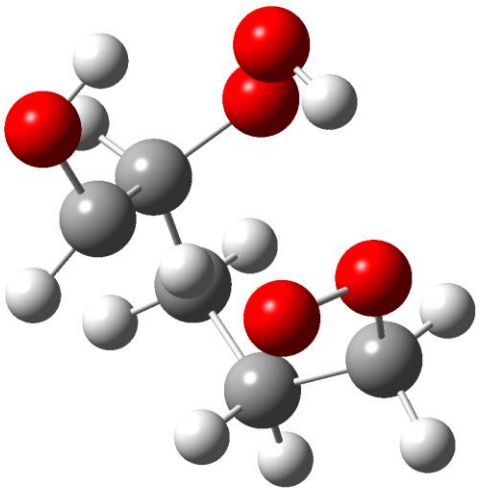
C 2.633157 -0.329790 -0.117778
H 3.151044 -0.360113 -1.077391
C 1.561079 -1.414243 -0.048236
C 0.296436 -1.038110 -0.827340
H -0.298426 -1.926660 -1.048205
C -0.567143 -0.071582 -0.042967
O 2.086323 0.984527 -0.088574
O 1.321799 1.128165 1.054513
H 1.986413 -2.334212 -0.449154
H 0.564882 -0.573783 -1.777162
H 0.281333 0.588356 0.702511
H 1.304696 -1.616712 0.992614
H 3.362207 -0.439772 0.687446
O -1.098589 0.848759 -0.935775
O -1.855468 1.820716 -0.229661
H -1.191968 2.509308 -0.079465
C -1.575429 -0.678699 0.910416
H -1.064454 -1.420632 1.523353
H -1.989768 0.086525 1.566736
O -2.592865 -1.358029 0.202764
H -3.084163 -0.710856 -0.311985

1,6 in ROOH_5OO P



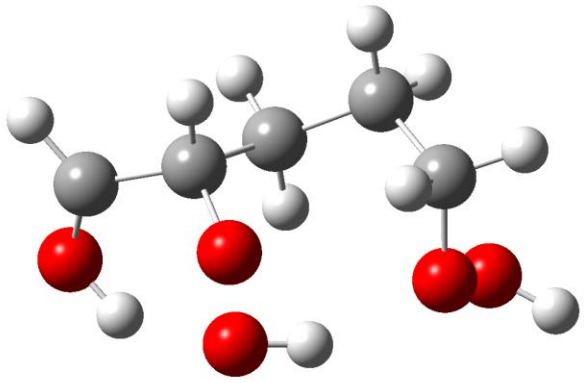
C -2.083325 0.199680 -0.636969
C 0.865803 0.462397 0.319719
H -3.098899 -0.128151 -0.410754
H -0.676440 -1.497733 0.914194
H -2.070932 0.661835 -1.627123
C -1.561683 1.166712 0.412413
H -1.613871 0.707572 1.399790
H -2.205027 2.046777 0.430615
C -0.124181 1.580429 0.114784
H -0.027411 1.968569 -0.901614
H 0.189083 2.379744 0.792465
O 0.804775 -0.303629 1.258548
O -1.428880 -1.756417 0.354732
O -1.245972 -0.933051 -0.785743
C 1.992027 0.340853 -0.672933
H 2.473582 1.320781 -0.771002
H 1.526419 0.113055 -1.641152
O 2.920884 -0.630444 -0.311442
H 2.565201 -1.084541 0.463742

1,7 in ROOH_5OO TS



C 2.134730 -0.378664 0.242164
C -0.705430 1.117152 0.204411
H 3.015626 -0.830099 -0.219679
H 2.338739 -0.183947 1.295639
C 1.779961 0.899228 -0.502112
H 1.565816 0.647728 -1.541418
H 2.695424 1.494124 -0.522636
C 0.664128 1.773767 0.076082
H 0.942948 2.129024 1.070290
H 0.558031 2.659092 -0.553664
O 0.590649 -1.584958 -0.980303
O 1.102300 -1.365083 0.282515
C -1.094762 0.311610 -1.021199
H -0.277627 -0.695364 -1.077087
H -0.859789 0.849861 -1.939794
H -1.475394 1.890907 0.316672
O -0.664595 0.383751 1.438614
O -1.386485 -0.833171 1.359021
H -0.657570 -1.447768 1.165629
O -2.384620 -0.137959 -1.071311
H -2.575952 -0.552754 -0.218318

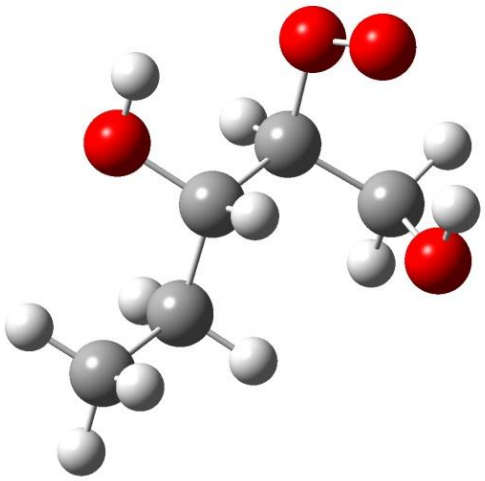
1,7 in ROOH_5OO P



C 1.954570 0.551549 0.723409
C -1.219514 0.684251 0.468007
H 2.984942 0.894947 0.844479
H 1.506903 0.401255 1.704155
C 1.156087 1.534723 -0.118991
H 1.754803 1.822519 -0.983045
H 1.018810 2.437490 0.482699
C -0.196255 1.028981 -0.619428
H -0.641346 1.802646 -1.246873
H -0.055592 0.163872 -1.269652
O 2.533696 -0.710269 -1.119157
O 1.968695 -0.768435 0.185107
C -2.591933 0.457329 -0.063800
H 3.377394 -1.158782 -0.983560
H -3.301027 1.269879 -0.115098
O -2.795932 -0.506478 -0.995017
H -2.160550 -1.215796 -0.825347
H -1.269819 1.498126 1.196545
O -0.770930 -0.414465 1.283574
O -0.695732 -1.583970 0.473070
H 0.249370 -1.588214 0.239906

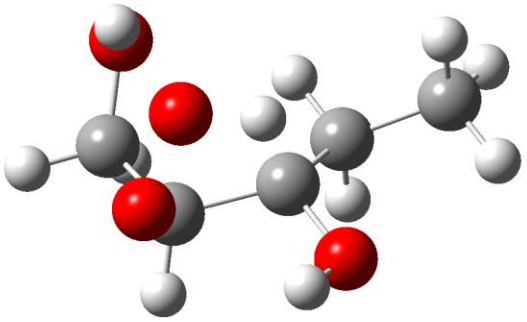
M06-2X/aug-cc-pVTZ calculated geometry coordinates for H-shift reactions peroxy radical HOCH2CH(OO)CR1HCH2CH3.

ROO_3OH



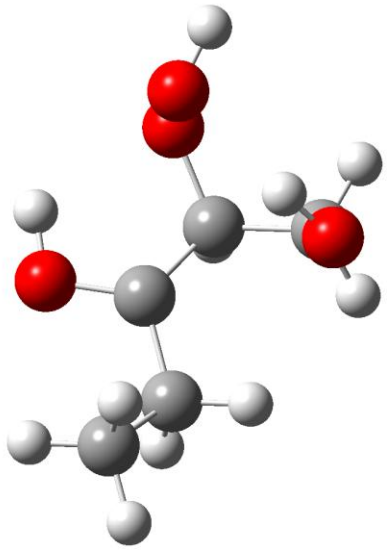
H 2.252357 1.192895 1.043552
C 1.223495 1.235228 0.672542
H 0.651235 1.865290 1.352780
C 0.634861 -0.165436 0.723955
C -0.640793 -0.368210 -0.085548
C -1.729443 0.598903 0.343740
H -1.363192 1.614138 0.190222
H -1.909831 0.463555 1.413985
C -3.020178 0.387389 -0.435908
H -2.850770 0.532643 -1.503649
H -3.782920 1.096216 -0.117411
H -3.400863 -0.620588 -0.287484
O 1.153257 1.842670 -0.594848
H 1.654748 1.294458 -1.206651
H 0.456399 -0.465820 1.757771
O 1.616219 -1.150825 0.277057
O 2.151050 -0.829975 -0.862395
H -0.403321 -0.199296 -1.141432
O -1.124195 -1.685308 0.107719
H -0.482147 -2.313229 -0.234639

1,4 in ROO_3OH TS



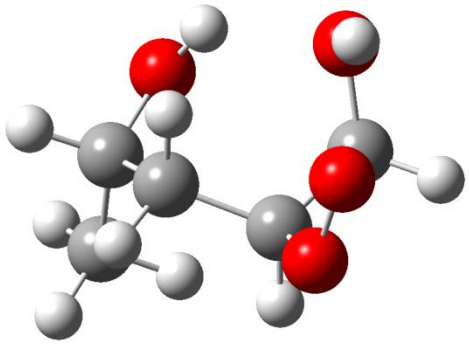
C -0.823464 -0.292013 -0.782833
C 0.600839 -0.360778 -0.190102
O -1.501038 -1.259057 0.011648
O -1.166769 -0.915390 1.329044
H 0.059425 -0.501352 0.976915
O 1.225857 -1.545450 -0.483509
C 1.534951 0.803796 -0.311809
H 0.999837 1.703242 -0.012880
H 1.798855 0.909372 -1.370891
C 2.800224 0.626528 0.521371
H 2.549406 0.520491 1.577083
H 3.451035 1.492200 0.414030
H 3.350584 -0.259887 0.213652
H -0.847256 -0.676511 -1.806618
C -1.470860 1.082182 -0.745031
H -2.511885 0.962187 -1.063040
H -0.971026 1.720884 -1.476021
O -1.389653 1.735573 0.498462
H -1.653894 1.105547 1.178828
H 0.577608 -2.259872 -0.425787

1,4 in ROO_3OH P



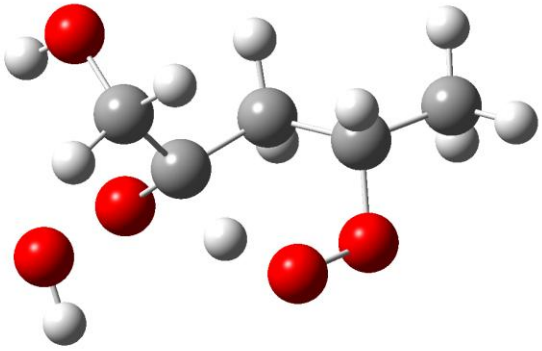
C 1.141029 1.334296 0.656044
H 2.214585 1.368684 0.872669
H 0.634373 1.942609 1.406131
C 0.687870 -0.111374 0.810764
H 0.716180 -0.368944 1.881831
C -0.651196 -0.409010 0.221075
C -1.823196 0.483314 0.422048
H -1.481065 1.516967 0.393269
H -2.251860 0.308518 1.419713
C -2.906422 0.262990 -0.632207
H -3.252147 -0.768811 -0.618313
H -3.758661 0.916067 -0.450121
O 0.850780 1.908923 -0.596309
H 1.032254 1.247222 -1.270826
O 1.655953 -1.046560 0.310151
O 1.865450 -0.759991 -1.078876
H -2.513387 0.475703 -1.626239
O -0.961734 -1.733049 0.138424
H -0.141228 -2.232022 0.045197
H 2.828865 -0.721874 -1.106761

ROO_4OH



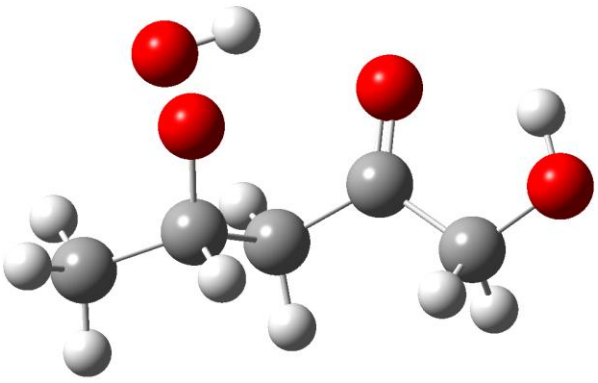
H	0.08202600	1.19941100	1.53216200
C	-0.78737600	0.87938700	0.96114700
H	-1.66287200	0.89971100	1.61572400
C	-0.55367400	-0.55368200	0.50425600
C	0.33597400	-0.71377900	-0.71874800
H	-0.13965800	-0.19737300	-1.55485000
C	1.77014800	-0.20885200	-0.55782800
H	2.27895200	-0.43438200	-1.50221100
C	2.52314800	-0.89698600	0.56633400
H	2.53394800	-1.97806900	0.42584900
H	2.06949100	-0.66762200	1.53125500
H	3.54988900	-0.53692400	0.59113500
O	-0.92856800	1.79696800	-0.10443200
H	-1.70105500	1.52660100	-0.61318900
H	0.37040300	-1.77396500	-0.97563900
O	1.84202700	1.18577300	-0.32001800
H	-0.18848900	-1.14543600	1.34390700
O	-1.83204700	-1.19889300	0.20954300
O	-2.57812400	-0.47750800	-0.56802000
H	1.05172900	1.62080200	-0.66168700

1,5 in ROO_4OH TS



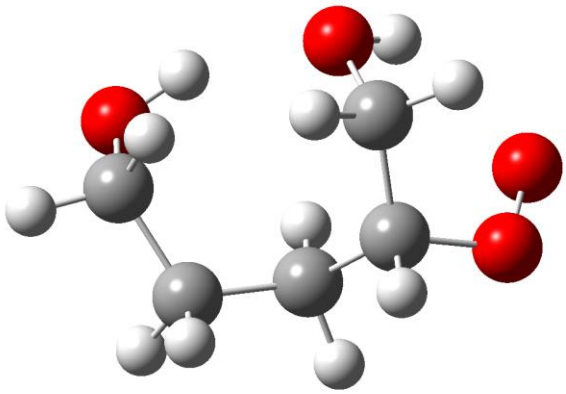
C -1.016890 -0.664667 0.773926
H -1.467079 -1.261696 1.569878
C 0.407979 -0.257661 1.185923
H 0.861506 -1.120069 1.672181
H 0.367979 0.559725 1.910461
C 1.293285 0.161210 0.016069
H 0.666423 -0.425354 -0.925811
O -0.920283 -1.583147 -0.308244
O -0.433164 -0.912943 -1.424199
C -1.966727 0.487859 0.484746
H -2.171508 1.010296 1.419609
H -2.906719 0.075661 0.109202
C 2.698129 -0.378113 0.029425
H 3.229590 0.004838 0.905011
H 3.231640 -0.056923 -0.862457
H 2.690638 -1.465533 0.073419
O 1.301226 1.507527 -0.269962
O -1.457691 1.457906 -0.415092
H -1.305342 0.997836 -1.250522
H 0.387509 1.834706 -0.221528

1,5 in ROO_4OH P



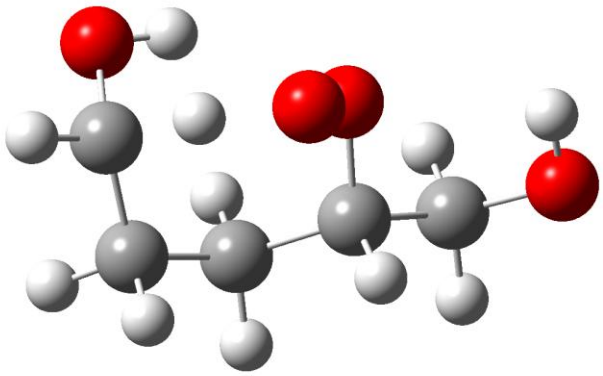
C -2.022757 -0.550636 0.578771
H -2.154124 -1.507580 1.084987
H -2.090207 0.246468 1.325291
C -0.651228 -0.508721 -0.069184
H -0.585543 -1.298282 -0.823135
C 0.486351 -0.652787 0.951795
H 0.462813 -1.675737 1.333104
H 0.307175 0.016168 1.795211
C 1.826758 -0.362807 0.372701
H 0.404042 1.925098 0.163533
C 2.347282 -1.136203 -0.786095
H 3.427977 -1.015751 -0.894564
H 2.142780 -2.198004 -0.655874
H 1.877835 -0.812346 -1.724828
O -3.048351 -0.441817 -0.379997
H -2.864607 0.341986 -0.907915
O 2.131173 0.985955 0.401552
O -0.513040 0.663937 -0.867132
O -0.542828 1.803599 -0.015628
H 2.937794 1.151501 -0.094099

ROO_5OH



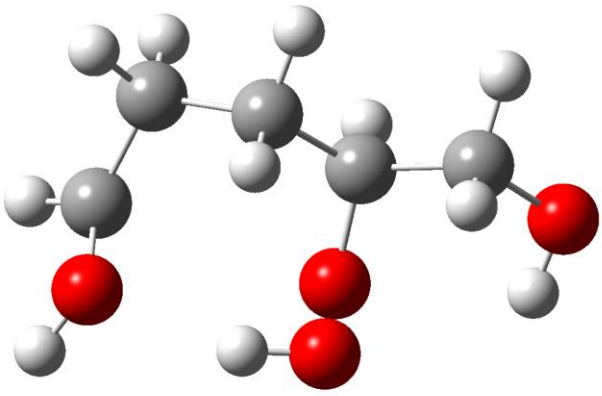
H 1.656666 1.192462 1.480957
C 0.715211 0.832725 1.056815
H -0.028419 0.837450 1.851038
C 0.915379 -0.598595 0.581499
H 0.996962 -1.257242 1.448260
C -0.107587 -1.132951 -0.407356
H 0.261313 -2.101072 -0.747936
C -1.521995 -1.308117 0.145075
H -2.064376 -1.942310 -0.557580
C -2.334415 -0.025090 0.321592
H -3.365556 -0.298197 0.548530
H -1.971916 0.564495 1.167494
O 0.249303 1.708849 0.051286
H 0.927667 1.729749 -0.633851
O 2.237190 -0.726801 -0.030900
O 2.472468 0.215832 -0.889783
H -0.129509 -0.479376 -1.280171
H -1.494557 -1.846451 1.097626
O -2.361694 0.762837 -0.846620
H -1.565969 1.306928 -0.831983

1,6 in ROO_5OH TS



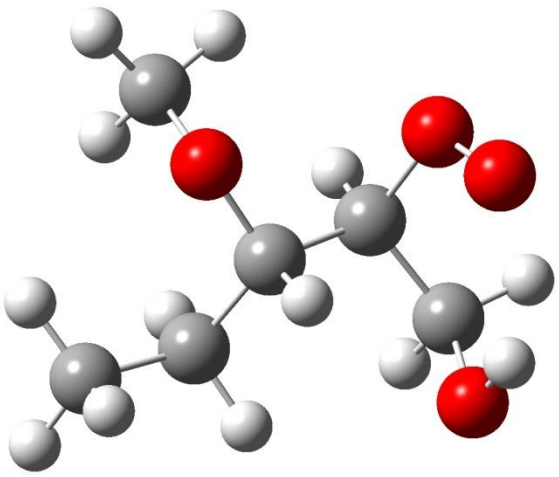
C 0.837195 0.343924 -0.317717
C -0.222651 1.394062 -0.029897
C -1.600488 1.105231 -0.633688
H -1.529675 1.067180 -1.722745
C -2.227718 -0.190806 -0.162035
H -3.206882 -0.400316 -0.587088
O 0.433994 -0.941495 0.187657
O -0.304772 -1.616446 -0.768901
H -0.312425 1.513391 1.054505
H -2.274883 1.928584 -0.381304
H -1.433969 -1.085360 -0.630659
H 0.132693 2.352909 -0.411794
H 1.009732 0.224212 -1.389448
O -2.261588 -0.400109 1.195786
C 2.149511 0.639656 0.382683
H 2.512831 1.617683 0.067879
H 1.976291 0.675186 1.465388
O 3.142976 -0.299463 0.055047
H 2.780981 -1.176926 0.214075
H -1.354661 -0.408847 1.528405

1,6 in ROO_5OH P



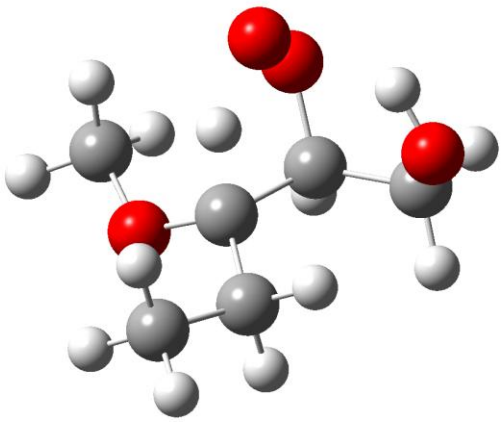
C 2.113441 0.553377 0.413579
H 2.420736 1.590370 0.550847
C 0.752062 0.517822 -0.262777
C -0.332824 1.144901 0.597540
H 0.033798 2.112374 0.945992
C -1.671351 1.358091 -0.114565
H -1.533615 2.016533 -0.974649
C -2.315656 0.112622 -0.597022
H -3.084972 0.137142 -1.357085
O 3.097259 -0.071651 -0.375511
H 0.819424 1.024445 -1.230528
O 0.450226 -0.820202 -0.664314
O 0.334577 -1.637088 0.495184
H -0.624106 -1.601647 0.647760
H 2.747628 -0.928807 -0.640333
H 2.037264 0.083485 1.399166
H -0.476797 0.534088 1.490138
H -2.342270 1.887213 0.577077
O -2.419763 -0.892893 0.341259
H -2.969516 -1.601406 -0.001862

ROO_3OCH3



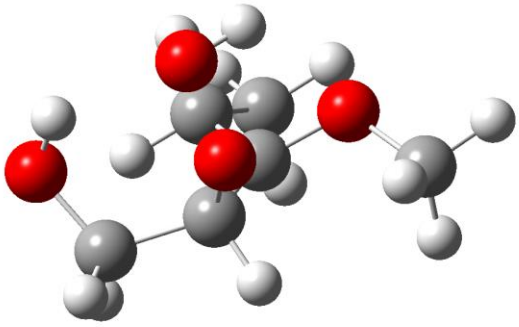
H 2.562512 0.577706 1.297588
C 1.627239 0.950325 0.868023
H 1.159188 1.602342 1.605178
C 0.708621 -0.240831 0.630852
C -0.482370 0.058917 -0.275016
C -1.326911 1.193474 0.304474
H -0.719129 2.098716 0.277919
H -1.556983 0.998909 1.356205
C -2.610115 1.405453 -0.486407
H -2.384298 1.603870 -1.534488
H -3.171730 2.251536 -0.093656
H -3.246813 0.522689 -0.451259
O 1.860651 1.735244 -0.275379
H 2.248363 1.161489 -0.944916
H 0.374451 -0.626680 1.595420
O 1.460087 -1.360456 0.088532
O 2.132867 -1.029928 -0.970187
H -0.092181 0.375178 -1.243215
O -1.229099 -1.104328 -0.565656
C -1.777048 -1.788759 0.536052
H -2.470390 -2.523452 0.134062
H -1.008529 -2.316840 1.108355
H -2.327000 -1.121176 1.206456

1,4 in ROO_3OCH3 TS



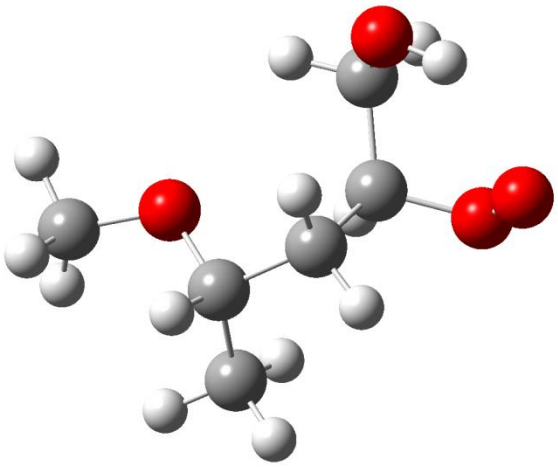
C -0.774357 -0.449531 -0.716030
C 0.558915 0.092982 -0.139474
O -1.160780 -1.463061 0.206044
O -0.914798 -0.919722 1.472270
H 0.125278 -0.212189 1.046138
O 1.662211 -0.655284 -0.428681
C 0.876619 1.556006 -0.290788
H 0.000220 2.131691 -0.001230
H 1.064527 1.751455 -1.352889
C 2.088233 1.977205 0.533771
H 1.912307 1.788122 1.593300
H 2.281367 3.041062 0.408445
H 2.977088 1.426787 0.234102
H -0.610367 -0.955922 -1.671992
C -1.869442 0.591825 -0.889792
H -2.745433 0.072888 -1.292973
H -1.550807 1.332498 -1.626109
O -2.197273 1.280270 0.292531
H -2.185994 0.647449 1.021122
C 1.594628 -2.056577 -0.205584
H 2.595328 -2.438519 -0.383068
H 1.285008 -2.260098 0.820929
H 0.889017 -2.534306 -0.885701

1,4 in ROO_3OCH3 P



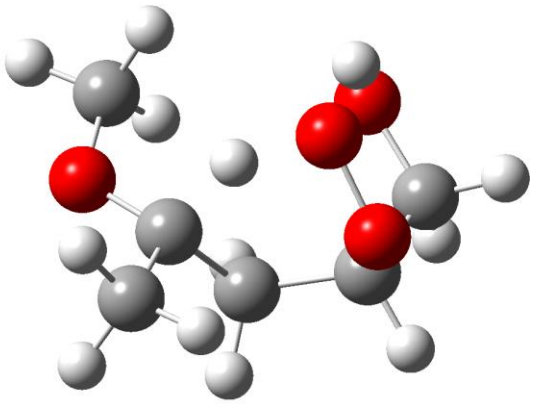
C -1.728922 -0.715401 1.029007
H -2.596819 -0.233330 1.489132
H -1.317653 -1.426803 1.748152
C -0.697780 0.369189 0.757806
H -0.571763 0.938220 1.687536
C 0.625010 -0.108112 0.245002
C 0.887973 -1.454000 -0.336063
H 0.648826 -1.439259 -1.409151
H 0.203456 -2.174900 0.104384
C 2.337690 -1.895738 -0.144442
H 2.580316 -1.962578 0.916620
H 2.502069 -2.873666 -0.594685
O -2.112703 -1.445627 -0.112129
H -2.206099 -0.831473 -0.847903
O -1.248954 1.392960 -0.101017
O -1.269986 0.921831 -1.443144
H 3.023986 -1.186727 -0.603295
H -0.366883 1.111593 -1.739307
O 1.452567 0.855138 -0.262245
C 1.643639 2.023803 0.524128
H 2.442452 2.586276 0.049198
H 0.738695 2.630901 0.558266
H 1.946360 1.748873 1.536715

ROO_4OCH3



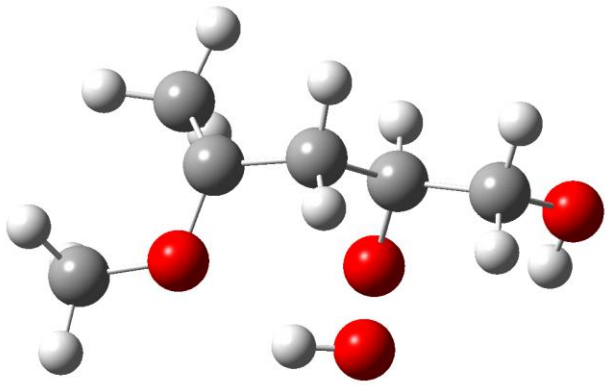
H	-0.42619700	1.90926600	0.73920700
C	-1.30405100	1.27766900	0.60981700
H	-1.93044300	1.35703500	1.50456200
C	-0.80686400	-0.15790700	0.49651400
C	-0.04224400	-0.45792400	-0.78964900
H	-0.29496100	0.29642300	-1.53294500
C	1.46610100	-0.47836100	-0.57044600
H	1.95375400	-0.46521700	-1.55369000
C	1.93822300	-1.71105200	0.18864900
H	1.66560500	-2.61137400	-0.36117700
H	1.48476300	-1.76128500	1.17906700
H	3.02013500	-1.71234100	0.31113200
O	-1.98219900	1.74137200	-0.53179500
H	-2.66909700	1.10404500	-0.75420100
H	-0.36024900	-1.42468800	-1.17937800
O	1.78960900	0.72460200	0.10861300
H	-0.20957400	-0.38176700	1.37958300
O	-1.93529400	-1.06799700	0.65728000
O	-2.78417300	-0.98234400	-0.32102500
C	3.16312500	1.02657000	0.14630600
H	3.25994900	2.04130200	0.52489600
H	3.71449500	0.35251600	0.80689600
H	3.60253700	0.97704900	-0.85568500

1,5 in ROO_4OCH3 TS



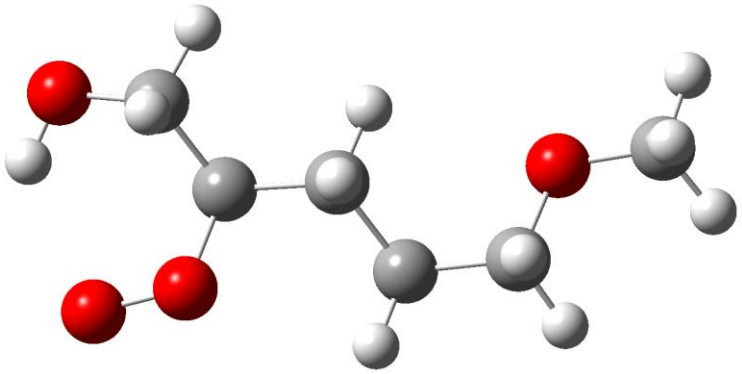
C 1.278034 0.704000 0.663290
H 1.734767 1.415400 1.352848
C -0.109126 0.260725 1.184915
H -0.403561 0.916105 2.005960
H -0.034407 -0.752386 1.573340
C -1.211033 0.323955 0.124763
H -0.490400 0.364673 -0.946355
O 1.130754 1.474867 -0.526782
O 0.601837 0.659284 -1.520630
C 2.245414 -0.457030 0.473732
H 2.551797 -0.813273 1.458417
H 3.133317 -0.082393 -0.045012
C -1.972902 1.621047 0.088196
H -2.539901 1.740764 1.015232
H -2.667444 1.631118 -0.748926
H -1.276837 2.453078 -0.006971
O -2.086297 -0.735473 0.071729
O 1.686492 -1.564023 -0.197301
H 1.396005 -1.242685 -1.057898
C -1.536904 -2.003210 -0.239356
H -0.776903 -2.315123 0.476307
H -2.363726 -2.707436 -0.230944
H -1.085904 -1.981999 -1.235375

1,5 in ROO_4OCH3 P



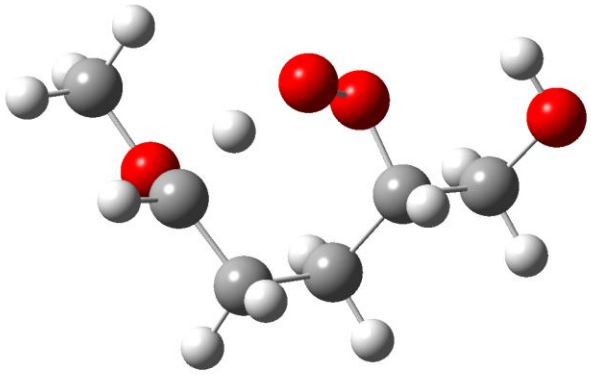
C 2.450207 0.339853 0.574790
H 2.719189 1.265988 1.083824
H 2.402377 -0.461288 1.318437
C 1.085833 0.495751 -0.070930
H 1.136831 1.282236 -0.829269
C -0.015979 0.808922 0.951341
H 0.155335 1.821424 1.323013
H 0.069921 0.128801 1.800353
C -1.390008 0.710986 0.380884
H -0.314840 -1.732525 0.194681
C -1.775122 1.569286 -0.776139
H -2.852478 1.714203 -0.855997
H -1.316057 2.550339 -0.663525
H -1.423014 1.140134 -1.724156
O 3.447366 0.086345 -0.387015
H 3.144506 -0.653714 -0.923196
O -1.869264 -0.578794 0.429709
O 0.779016 -0.648712 -0.862887
O 0.635376 -1.775845 -0.005832
C -3.196670 -0.785060 -0.017437
H -3.282818 -0.623817 -1.092830
H -3.446663 -1.816853 0.212786
H -3.881808 -0.117305 0.509029

ROO_5OCH3



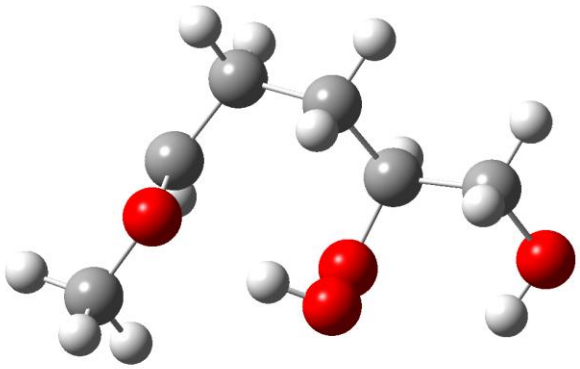
H -1.614271 2.204869 0.173259
C -2.137710 1.263234 0.340901
H -2.251014 1.127885 1.423454
C -1.268629 0.136569 -0.191486
H -1.351038 0.079103 -1.278793
C 0.169626 0.225824 0.268620
H 0.191424 0.248638 1.362441
C 1.041653 -0.913380 -0.246595
H 0.665582 -1.870884 0.115575
C 2.483576 -0.760062 0.186966
H 2.552152 -0.737055 1.283835
H 3.082298 -1.609389 -0.164245
O -3.382666 1.369713 -0.301526
H -3.779099 0.492587 -0.336219
O -1.772439 -1.132981 0.322787
O -2.946740 -1.431297 -0.140684
H 0.575802 1.175339 -0.080643
H 1.003932 -0.939180 -1.338164
O 2.993250 0.439765 -0.346390
C 4.332585 0.661332 0.015770
H 4.648381 1.596651 -0.439791
H 4.977610 -0.148336 -0.342642
H 4.440394 0.737078 1.103384

1,6 in ROO_5OCH3 TS



C 1.276650 -0.368964 0.190300
C 0.325915 -1.440677 -0.321429
C -0.939968 -1.650471 0.516406
H -0.674548 -1.889422 1.548230
C -1.839223 -0.443703 0.535959
H -2.692492 -0.497165 1.221597
O 0.681342 0.935250 0.159582
O -0.074058 1.142833 1.296856
H 0.042255 -1.191807 -1.345556
H -1.495603 -2.503964 0.117909
H -1.094997 0.476216 1.052881
H 0.877310 -2.382744 -0.356697
H 1.582882 -0.560938 1.222317
O -2.179812 -0.036991 -0.724204
C 2.505337 -0.236265 -0.690497
H 3.022384 -1.194261 -0.736544
H 2.186334 0.027884 -1.705674
O 3.418055 0.706043 -0.181216
H 2.929582 1.517067 -0.008887
C -2.978812 1.130106 -0.750450
H -2.432042 1.968808 -0.313335
H -3.207047 1.341011 -1.790872
H -3.907639 0.972072 -0.195254

1,6 in ROO_5OCH3 P



C 2.534946 0.217707 0.344574
H 3.091214 1.154064 0.389535
C 1.171986 0.474259 -0.279175
C 0.312976 1.400428 0.564590
H 0.908938 2.280341 0.815869
C -0.987368 1.862687 -0.116490
H -0.746065 2.473577 -0.987718
C -1.882972 0.768077 -0.567545
H -1.859344 0.394952 -1.584912
O 3.294809 -0.681268 -0.427295
H 1.310627 0.883004 -1.284944
O 0.532206 -0.773932 -0.566072
O 0.285654 -1.462294 0.654311
H -0.609571 -1.145734 0.863528
H 2.741142 -1.449973 -0.598685
H 2.400755 -0.151771 1.366100
H 0.082735 0.907937 1.510587
H -1.523766 2.507839 0.585899
O -2.211714 -0.149613 0.389157
C -3.031468 -1.204984 -0.090531
H -2.505194 -1.764651 -0.867768
H -3.244730 -1.857416 0.751716
H -3.962996 -0.804355 -0.492548